Preliminary Design Report

Inelastic X-ray Scattering CDT

Sector 30

Prepared by IXS-CDT Design team:
M. Ramanathan
B. Brajuskovic
D. Shu
Y. Amer
H. Sinn
C. Burns (WMU)
W. Sturhahn
T. S. Toellner
E. E. Alp
J. Hill (BNL)

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Table of Contents

1 Scientific Objective of the IXS CDT

The IXS-CDT intends to build two separate inelastic x-ray spectrometers to study collective excitations in condensed matter. One of these spectrometers aims to study collective valence electron excitations in correlated electron systems, primarily of transition-metal oxides. The energy range is 5-12 keV, and the targeted energy resolution is around 100 meV. The instrument is named the medium-resolution inelastic x-ray spectrometer (MERIX) due to its relatively moderate-resolution factor of 10^5. The second spectrometer is designed to study collective excitations of atoms, ions, molecules or polymer etches in crystals and more importantly in disordered systems, such as liquids and biological systems such as a lipid membrane, proteins, DNA and amorphous solids. This instrument is called the high-resolution inelastic x-ray spectrometer (HERIX). The energy range is 21-26 keV, and the resolution factor exceeds 10^7.

Inelastic x-ray scattering (IXS) experiments require highly complex setups, with high-resolution secondary monochromators and backscattering analyzers. The experiments are usually conducted with low count rates of a few Hz. These requirements make time-sharing with other experiments extremely inefficient. Without a dedicated setup, a large amount of beam time would be wasted in each experimental period, and, inevitably, compromises are made with the beamline optics, which prevent the most efficient use of the source. In addition, such time-sharing practices restrict the technique to the small fraction of the (x-ray) community who are willing or able to construct such an apparatus. At the very high-resolution (few meV) level, time-sharing is totally impractical, and only a dedicated instrument with associated beamline scientists, such as dedicated beamlines ID 28 at the ESRF (France) and BL35XU at SPring-8 (Japan), has any chance of success. As a result of these considerations, IXS-CDT was formed to design, build and operate a beamline focused on this single technique. The goal is to produce a reliable, state-of-the-art, user-friendly beamline that would be made available to a wide community.

The IXS-CDT members come both from the existing inelastic x-ray scattering community and from the broader scientific community that would like to have access to such an instrument but lack the expertise or resources to operate one. They share the common belief that inelastic x-ray scattering can address some of the important problems in their fields. As a result, IXS-CDT has an extremely broad scientific program, ranging from condensed matter physics, to polymer science to biology. The CDT members bring significant resources to the consortium. These include optics and instrumentation development from the Argonne and Brookhaven groups and the long expertise in inelastic x-ray scattering from some of the pioneers in the field. Existing funding consists of $900,000 from the NSF over 3 years (2002-2005) to build the high-resolution instrument (HERIX), matched by $550,000 from member institutions. In addition, IXS-CDT has $5,000,000 from the DOE over 5 years, 2002-2007 for the beamline and the medium-resolution instrument (MERIX), and commitments from the APS for the undulators, vacuum chambers and front-ends. Finally, the APS will be providing significant assistance in the design, procurement and operational aspects of the CDT through the assignment of APS personnel to IXS-CDT responsibilities, including front-end, specialized undulators, the implementation of the extended straight section and the hiring of beamline scientists and other operational staff.

2 Rationale for the Choice of Insertion Devices

The choice of insertion devices (IDs) is based on the tunability over the required energy range, and the IDs are optimized for maximum flux per unit power generated. In addition, constraints, such as minimum gap allowed, maximum power that can be handled in the front-end, are part of the optimization process. However, the underlying goal is to deliver approximately 5-10 times more spectral flux (photons/see/eV) in the energy range targeted than currently available.

In addition, all energy ranges must be accessible all of the time. Due to relatively large difference in the range of MERIX and HERIX instruments, we consider the following scenario as optimum.

- permanent magnet undulators (PMU) with a period of 3.0 cm with each 2.5 m length, a total of 2 or 3 devices, plus superconducting undulator (SCU) with a period of 1.45 cm and a total magnetic length of 2.5 m.

In order to place all four undulators at a given straight section, the length of the straight section must be extended to 12 m. A study has been conducted by the APS (all three divisions were involved) showing that, from an accelerator performance point of view, either an extension to 8.5 m or 12 m is possible. A cost estimate also has been made and presented to the APS director. At the time of the writing of this report, no decision has been made as to whether any of these options will be accepted. Our expectation is that a 12 m extension will ultimately be chosen, but it is possible to implement this in two steps rather than at once.

The second important issue is the availability of a SCU. The APS commissioned a study to answer some of the questions regarding minimum gap, cooling systems, reliability and cost. The report of this study is expected in the spring of 2004. Given the uncertainties in the length of the straight section and availability of a SCU, we adopt the following strategy.

- Start commissioning with one 3.0 cm PMU in October 2004.
- Acquire a second 3.0 cm PMU by spring 2005.
- Implement an extended straight section by summer 2006, and add a third 3.0 cm period PMU.
- If SCU study and cost estimates are favorable, place an order in CY 2004.
- Have the ideal solution of 3 PMU and 1 SCU by 2007.

We believe that this plan is realistic, facilitates development of the beamline, and allows us to reach the original goal of simultaneous access to 5-12 keV and 21-26 keV range in the first harmonics of a PMU and SCU, respectively.

The expected brilliance of these devices and total power generated are given in Figures 2.1 and 2.2. Note that a new front-end with power handling capability of 21 kW is being implemented. Also, the energy range mentioned above can be reached with a gap of 10.5 mm for the PMU and 7.5 mm clear gap for the SCU.

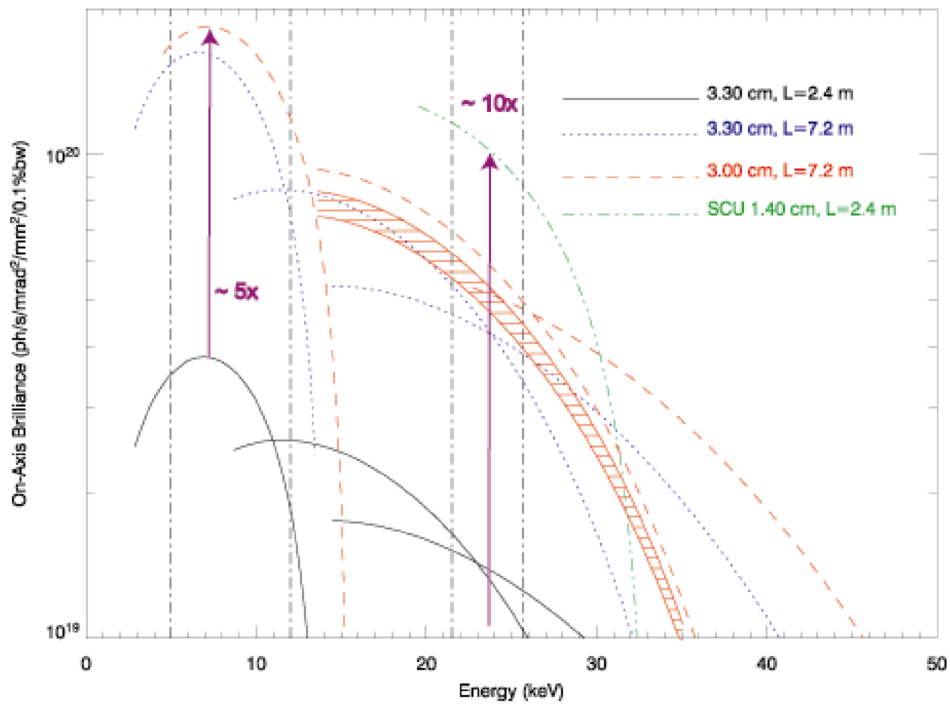


Figure 2.1 *Calculated performance of permanent magnet and superconducting undulators at a ring current of 100 mA. The hatched area is a realistic brilliance expected from the third harmonics.*

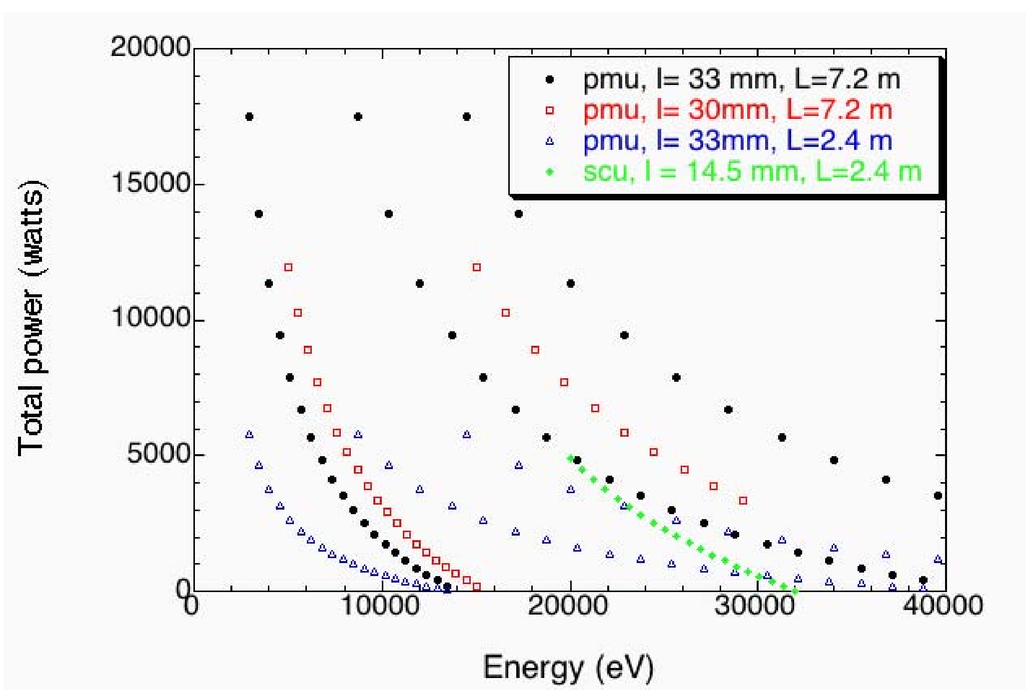


Figure 2.2 *The total power generated for the PMU and SCU as a function of energy. The calculations are for a ring current of 100 mA.*

As can be seen in Figure 2.1, the expected brilliance increase is a factor of 5 at 8 keV for 3 PMUs (3.0 cm period) over the existing, single current standard undulator A device (3.3 cm period). The expected increase at 25 keV is about an order of magnitude from today, and a factor of 2 higher from the combined performance of 3.0 cm devices. Another advantage is, of course, reduced total heat load when the SCU is used, and this allows the possibility of accommodating higher current operations.

Finally, the proposed combination of undulators is compatible with the new front-end at 150 mA operations when all device gaps are closed.

3 Sector Layout

The IXS-CDT intends to develop and build the insertion device beamline. However, provisions have been made to ensure that a bending magnet beamline can also be built. Appendix A figure A.1 shows an overall layout of the sector along with a possible bending magnet beamline.

The ID beamline, designed to satisfy the scientific program outlined elsewhere, will carry out experiments in two different regimes:

- Medium-energy-resolution experiments in the 5-12 keV region with approximately 100 meV resolution. This spectrometer has been dubbed MERIX. Experimental requirements include an energy-tunable beamline and horizontal and vertical diffraction capabilities for polarization selection. In particular, most of the transition-metal K edges need to be covered.

- High-energy-resolution experiments with sub-meV resolution with an incident energy in the 21-26 keV region. This spectrometer has been dubbed HERIX. It is designed to reach sub-meV resolution (~1 ± 0.1 meV) and an adequate momentum-transfer range (0.05 – 6.7 $Å^{-1}$).

It is not possible to design a single insertion device that is optimized for both energy ranges. We have therefore chosen to work with two separate types of devices, each optimized for the appropriate regime. The proposed beamline is composed of three stations, including the two end stations, as shown in Figure A.2. This design enables the setting up of experiments in the HERIX station, while conducting experiments in the MERIX station. In addition, during the HERIX experiments, the high-resolution monochromators will be completely isolated, so that the required thermal stability can be reached.

Note, the high incident energy of the high-resolution spectrometer is dictated by the energy-resolution requirement. The preferred method of energy analysis is to use a back-scattering bent silicon analyzer, which determines the achievable resolution. There is a reverse correlation between the incident energy and maximum achievable resolution. In order to reach the sub-meV level, the incident energy must be higher than 22 keV. The potential choices for analyzer reflections with adequate reflectivity (R > 60 %) are given in Table 3.1. Therefore, we plan to design an undulator with a short enough period, consistent with the minimum achievable gap at the APS, to give a first harmonic in the range of 21-26 keV.

Table 3.1 *The possible reflections for the IXS-CDT HERIX instrument, and corresponding energy, intrinsic energy resolution, and room temperature reflectivity of the analyzer without the geometry, source size and incident energy band-pass contributions. These contributions can be kept at a minimum to achieve an overall resolution of ~1 meV for the energy range of 22-25 keV, while maintaining a reasonable reflectivity and throughput.*

Si Reflection at 90°	**Energy (keV)**	**Resolution (meV)**	**Reflectivity (%)**
18 6 0	21.657	1.23	78
11 11 11	21.747	0.83	70
13 11 9	21.985	0.81	69
15 11 7	22.685	0.70	68
20 4 0	23.280	0.87	76
12 12 12	23.724	0.80	75
14 14 8	24.374	0.69	74
22 2 0	25.215	0.576	71
13 13 13	25.701	0.37	60

3.1 Front-End Layout

The front-end design is the responsibility of the APS. Due to the special needs of the IXS-CDT beamline, the XFD Engineering Group has designed a new front-end to handle a total power of 21 kW and a maximum normal incidence peak power density of 2100 W/mm^2 at about 17.2 m from the center of the straight section. The IXS-CDT beamline only requires a 1x3 mm aperture at the entrance to the first optics enclosure (FOE). In addition, IXS-CDT would like to operate the beamline with a Be window. The new front-end has been designed based on these criteria.

3.2 Beamline Layout

The basic beamline philosophy is to achieve straightforward and reliable operation. Based on the first 5 years of experience of APS operations, we have decided to implement the following structure:

- Tandem undulators, separately optimized for HERIX and MERIX
- A white beam Be compound-refractive lens (CRL) to collimate the beam for increased performance of the downstream optical elements
- A water-cooled diamond double-crystal high-heat-load monochromator
- Channel-cut silicon monochromators for the MERIX spectrometer
- An "in-line" cryogenically cooled, energy-tunable monochromator for the HERIX spectrometer
- Kirkpatrick-Baez (K-B) focusing mirrors
- MERIX and HERIX spectrometers - housed in separate stations

Station A (FOE) is a white beam station and houses the white beam optics and the high-heat-load monochromator. The FOE houses the beam-defining components, like the slits and a white beam refractive lens for collimation; in addition, it houses the bremsstrahlung stop and a monochromatic photon shutter. Station B (MERIX) is a monochromatic station and houses the high-resolution monochromators followed by K-B focusing mirrors for the MERIX. The MERIX spectrometer is placed in this station. The monochromatic photon shutter for the next station is located here. Station C (HERIX) is also a monochromatic station, houses K-B mirrors and the HERIX spectrometer. A work-area enclosure is planned to encompass the two monochromatic stations for operating the beamline.

3.2.1 Survey and Alignment Plans

All beamline components will be surveyed and aligned in place by the APS Survey and Alignment Group. In order to facilitate ease in alignment, all components will be fiduciallized to external reference points on their table during assembly. All components are designed with a liberal tolerance allowance of greater than 0.5 mm.

3.2.2 Utility Layouts

The beamline utilities layout is shown in figure A.3 in appendix A. The sector is supplied with two 30 KVA 3 phase transformers located at the end of the sector to provide for clean and utility power for the beamline. In addition, limited capacity of 120 VAC emergency power is available. All emergency power outlets will be colored red, and there will be one duplex outlet in each station and one on top of the stations. Each station is equipped with a dedicated labyrinth for the mechanical piping. Each station has two 1" stainless-steel (SS) pipes for the de-ionized water, two 1" SS insulated pipes for chilled water and a ¾" copper pipe for air. The station doors will also be supplied with air for operation. The air for the whole beamline is house air and will be connected together with 1" copper piping. The de-ionized water lines from the stations will be tied together with 2" SS piping as shown in the layout. The de-ionized water for the beamline is provided by the APS. Isolation valves will be provided in the main lines prior to connection to the APS system water in the mechanical mezzanine. The chilled water will be distributed to the stations via 2" SS insulated pipes. The water for the chilled water will be de-ionized water, which will be chilled with a heat exchanger in the mechanical mezzanine. The APS-provided chilled water will be used in the mechanical mezzanine for the heat exchanger. The design of the utility distribution is being done in consultation with the ASD Mechanical and AOD Conventional Facilities Groups.

3.2.3 Life Safety Code Compliance

Figure A.1 in appendix A shows a layout of the sector with the aisle way and access points clearly marked. The IXS-CDT beamline consists of three contiguous stations. The aisle way between sectors 30 and 31 is a dead-end pocket as shown in layout. In compliance with the Argonne Life Safety Codes, an access corridor is established behind station C and will be clearly marked with yellow tape for identification purposes. Access to the stations roofs is via a ladder located at the end of station C. There are transition steps between station C and B and to the roof of the storage ring.

3.2.4 Beamline Vacuum System

The beamline has been designed in full compliance of the APS vacuum policy. All beamline components are designed to ultrahigh vacuum (UHV) standards. The beamline is expected to operate in high vacuum (HV). The beamline will use Gamma One (former Physical Electronics) ion pumps for the vacuum pumps and will use Televac cold cathode and convectron gauges for monitoring. Turbo pumps backed up by oil-free pumps will be used for the pumping stations. All gate valves will be APS standard VAT style valves. A rough vacuum system for each of the experiment stations is planned for use in pumping sample chambers, flight paths, etc.

3.2.5 Data Acquisition System and Motion Control

The control system of choice for the beamline will be EPICS based. The beamline will employ mainly Sun-based Solaris machines and also INTEL-based Linux machines. The beamline hardware for motion control will be VME based. The APS Beamline Control and data Acquisition (BCDA) Group software will be used for the control of the beamline. In addition SPEC software package will be installed. Other user-friendly software will be installed as needed. All the computers will be linked via hard-wired Ethernet to the APS central network. The network and the computers will be configured and maintained by the APS Information Technology (IT) Group.

3.3 Beamline Components

The plan and elevation layout of the beamline components is shown in figure A.2 in appendix A. Appendix B is a table of the beamline components along with their positions along the beamline.

One of the consequences of tandem operation of undulators at IXS-CDT is increased heat load on the beamline components that are exposed to white beam. Although the small size of the exit-mask opening (3 mm x 1 mm) limits the total heat load to the levels that are customary for the beamline components, the surface density of the load is increased considerably, and the design of beamline components exposed to the white beam has to be re-evaluated.

The beamline employs mostly APS standard components. When needed, modifications to the standard components have been made, and their associated thermal calculations were performed. Listed below are descriptions of the key beamline components and associated thermal analysis.

3.3.1 White Beam Slits

The beamline has a white beam slit to define the beam prior to incidence on the white beam lens and the monochromator. The design of the white beam slits is based on the design and operation experiences from the APS XOR 3-ID white beam slits.

The white beam slit (1403300702-940000-00-1 or L5-94v0) is a modified design of the 3-ID pseudo-knife-edge white-beam slit L5-92v5. Figure A.4 is an assembly drawing of the slit and focusing lens systems. It uses a Glidcop/SS explosive-bonding unit for its water-cooling mask. A tungsten knife-edge block is mounted downstream of the cooling mask to define its 0 – 4.4 mm x 0 – 4.4 mm optical aperture. The major modification of the L5-94v0 is its cooling-surface grazing-incidence angle. Instead of a 1.83 degree grazing-incidence angle for both horizontal and vertical cooling surfaces in the L5-92v5 design, the L5-94v0 has 0.97 degree and 0.75 degree grazing-incidence angles for its horizontal and vertical cooling surfaces, respectively, which will provide more than enough thermal-load-handling capacity compatible with new front-end design for this beamline.

3.3.2 Collimating Lens

Following the white beam slit is a white beam compound refractive lens to collimate the white beam divergence. The design is based on the design and operation experiences from the APS XOR 3-ID beamline. This lens is needed because the angular acceptance of diamond falls below the opening angle of the undulator radiation above 15 keV, as shown in figure 3.1.

Consistent with that for the white beam slits, a similar design modification was also applied to the white beam collimator for the IXS-CDT white beam compound refractive lens. A 0.8 degree grazing-incidence angle (instead of 3 degrees used in the 3-ID original design) has been used in the new design. The other modification to the white beam compound refractive lens is its optimized photon energies for the beam collimating. Two photon energies (26 keV and 22 keV) have been chosen for the new lens design. The lens when translated has a clear aperture for beam to pass through when operating at lower energies for MERIX.

In figure 3.1, the horizontal straight line indicates the approximate opening angle of undulator radiation at the APS. Therefore it is useful to have a collimating compound refractive lens (CRL) to improve the efficiency of the monochromator for energies above 15 keV. Sector 3 implemented a Be CRL two years ago, and the operational experience has been a positive one (J.Y. Zhao, E.E. Alp, T.S. Toellner, W. Sturhahn, H. Sinn, and D. Shu. Rev. Sci. Instrum. **73** (2002) 1611-1613.)

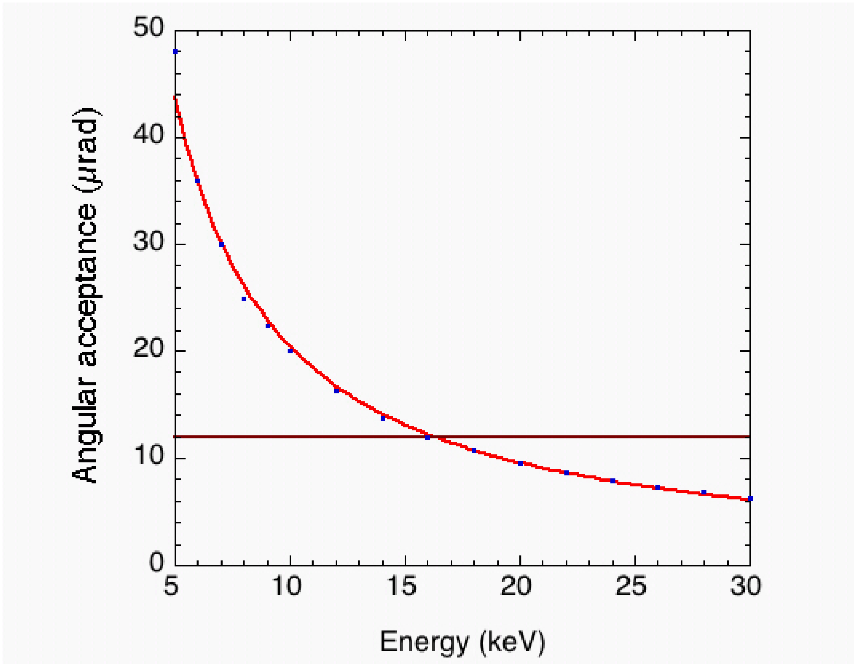


Figure 3.1 *The angular acceptance (i.e., Darwin width) of the diamond (111) reflection as a function of energy.*

3.3.3 High-Heat-Load Monochromator

The high-heat-load monochromator will be a double-crystal water-cooled diamond. The angular acceptance of diamond at 30 keV is around 6.3 microradians. The opening angle of the undulator radiation is typically around 12 microradians. However, there are published reports that this divergence can be reduced to under five microradians. Currently, a white-beam-collimating Be compound refractive lens is installed at sector 3 of the APS. The performance of the lens has encouraged us to use the diamond high-heat-load monochromator. Appendix C is the statement of work used for the procurement of the high-heat-load monochromator (HHLM).

3.3.4 Integral Shutter

Figure A.5 is an assembly drawing of the integral shutter P5-80. This shutter is based on the APS standard component P5-70 used in sector 1. The higher heat-load requirements for this beamline necessitate a new mask design for the integral shutter. The integral shutter is located at the end of the A station. The design of the new mask is modular and fits into the existing design of the rest of the P5-70 shutter. The new mask is made to handle increased heat-load densities.

The thermal load distribution in the plane normal to the beam axis was calculated by Yifei Jaski using the program SRUF. Calculations were made for three undulator A units positioned upstream in the straight section, with 150 mA current, and the gap set to obtain a **k** value of 2. It was assumed that if the lineup of the undulators is later changed, the total thermal load of the beam will be held lower or at the level of the thermal load calculated for this case. The thermal load distribution was calculated as:

$$Q_{(x,y)}=e^{(5.1712-0.029457X^2-0.33066Y^2)}+e^{(5.3357-0.035664X^2-0.38677Y^2)}+e^{(5.5149-0.043808X^2-0.46025Y^2)} \quad [W/mm^2]$$

and the distribution of the portion of the load that goes through the exit mask is given in figure 3.2.

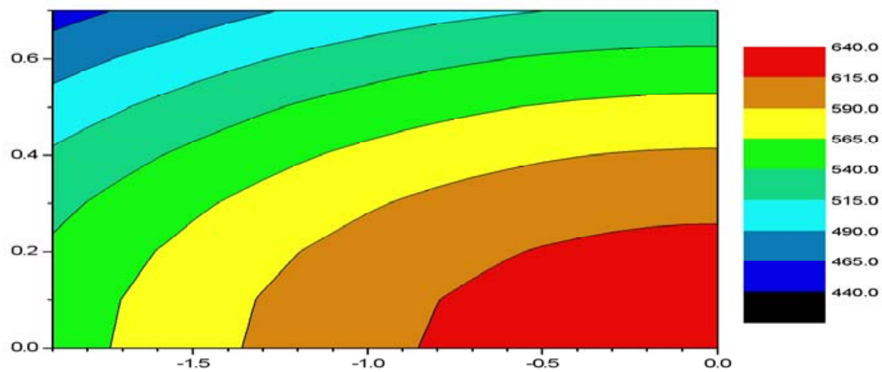


Figure 3.2. *Thermal load distribution in the plane perpendicular to the beam axis and at 30.3 m from the center of the straight section (lower right quadrant).*

The calculated total power absorbed by the white beam stop is 2.5 kW, while the peak heat flux is 640 W/mm^2. The increase in the thermal load density at this beamline was countered by decreasing the beam stop incidence angle from 4.5° to 1.55° (figure 3.3a), which in turn leads to an increase in the beam stop length of 7". Also the entrance and exit openings of the mask body were redesigned in order to provide masking of the white beam even in extreme cases of beam misalignment. Figure 3.3 (b) is a cross-sectional view of the mask with the beam footprint (3mm x 5mm), taking into account beam misalignment.

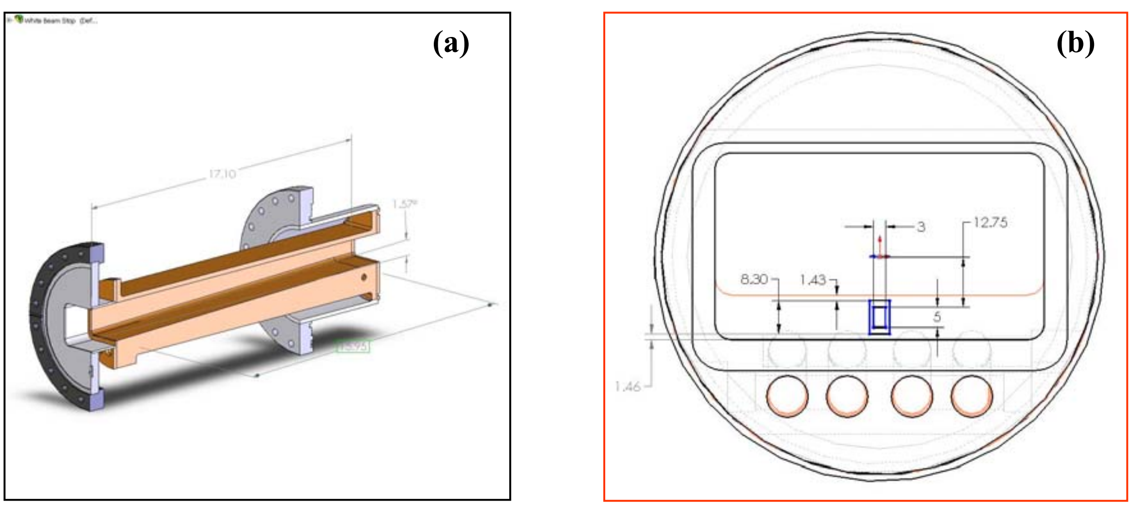
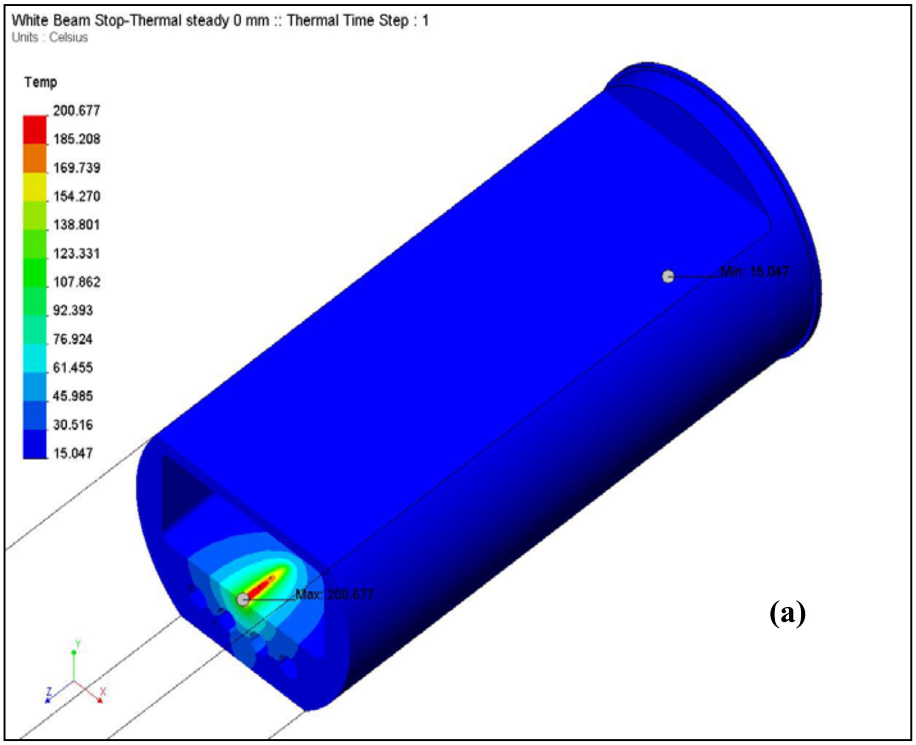
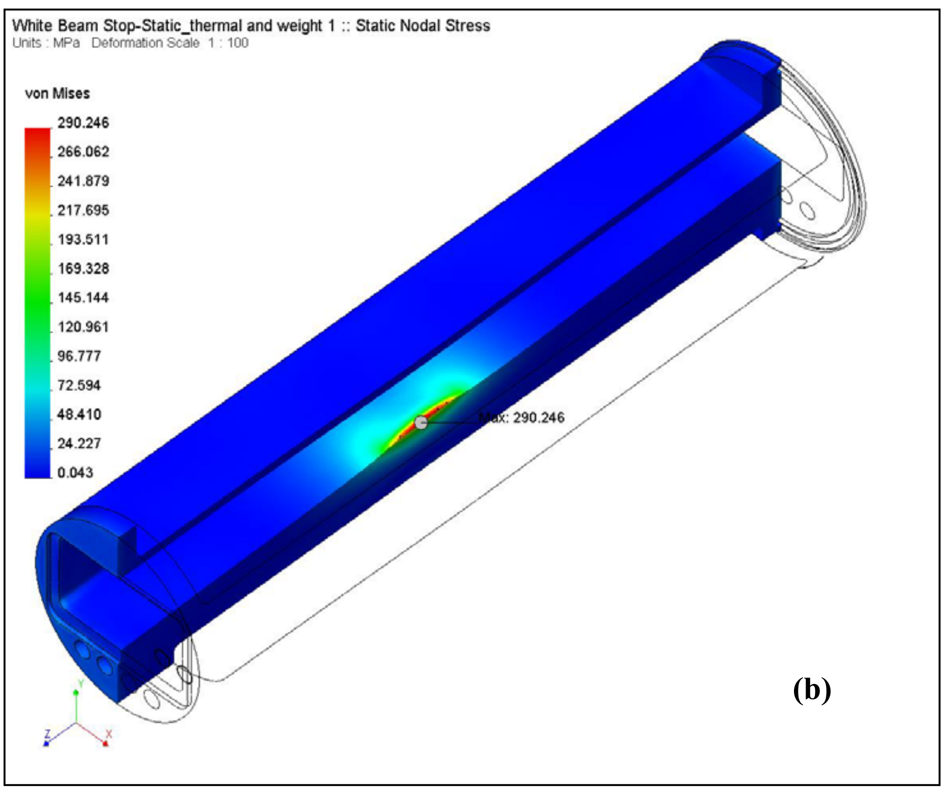


Figure 3.3 *(a) Cutout view of the 1.5° incidence angle white beam stop, and (b) cross-section view with the beam footprint.*

Extensive finite element analysis (FEA) calculations show that, under normal operating conditions, the temperatures and thermally induced stresses will stay within the acceptable range, as shown in figure 3.4.



(a)



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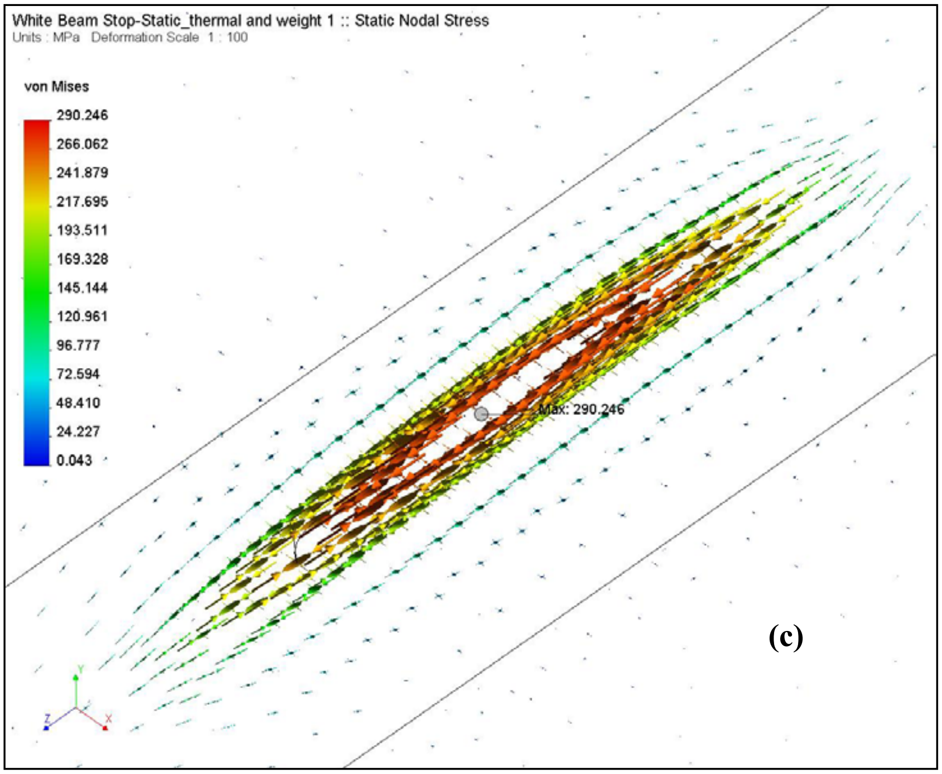
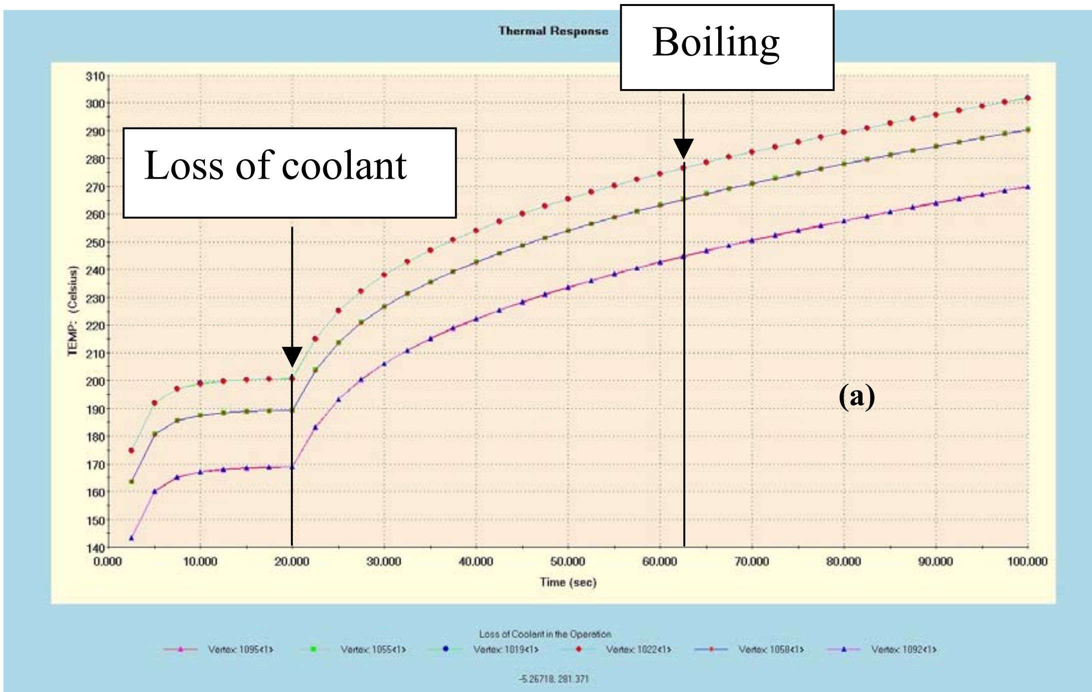
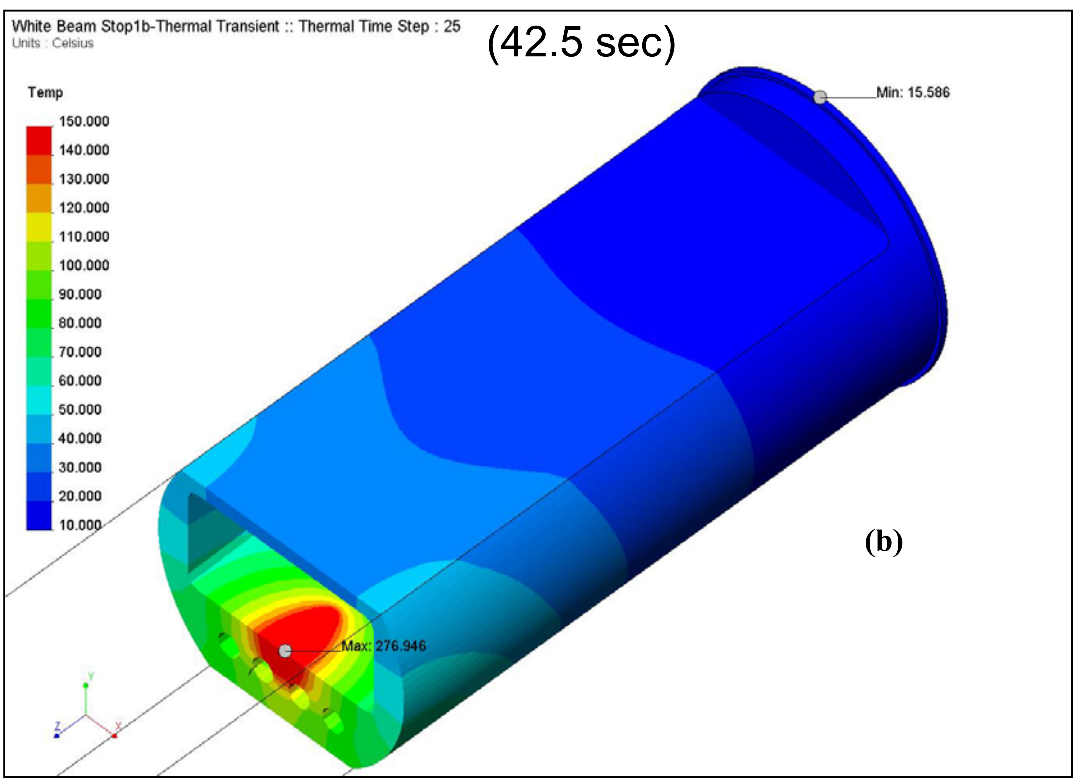


Figure 3.4 *FEA results for normal operating conditions: (a) temperature distribution, (b) stress distribution, and (c) stress orientation.*

The highest temperature calculated for normal operating conditions is 200°C. It is important to note that temperatures of the cooling channel walls (<75 °C) stay way below the boiling point temperature of the cooling water. Maximum calculated stresses are below 300 Mpa, and the material in the footprint area is stressed into compression.

The influence of beam misalignment and loss of coolant were investigated through a number of scenarios. Results of the analyses show that beam misalignment has only a minor effect on both calculated temperature and stress levels. Total loss of coolant is a catastrophic event. The results of the transient analysis, as shown in figure 3.5, indicate that, approximately 45 seconds after total loss of coolant, the temperature of the cooling channel walls exceeds the boiling temperature. At that moment, stresses are in the plastic region but lower than the ultimate strength of Glidcop. Temperatures and stresses continue to rise in time, but the heat transfer conditions are not accurately described in this model and results are not accurate.


Thermal Response
Boiling
Loss of coolant
TEMP: (Celsius)
Time (sec)
(a)
Loss of Coolant in the Operation


White Beam Stop1b-Thermal Transient :: Thermal Time Step : 25
Units : Celsius
(42.5 sec)
Temp
150.000
140.000
130.000
120.000
110.000
100.000
90.000
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40.000
30.000
20.000
10.000
Min: 15.586
Max: 276.946
(b)

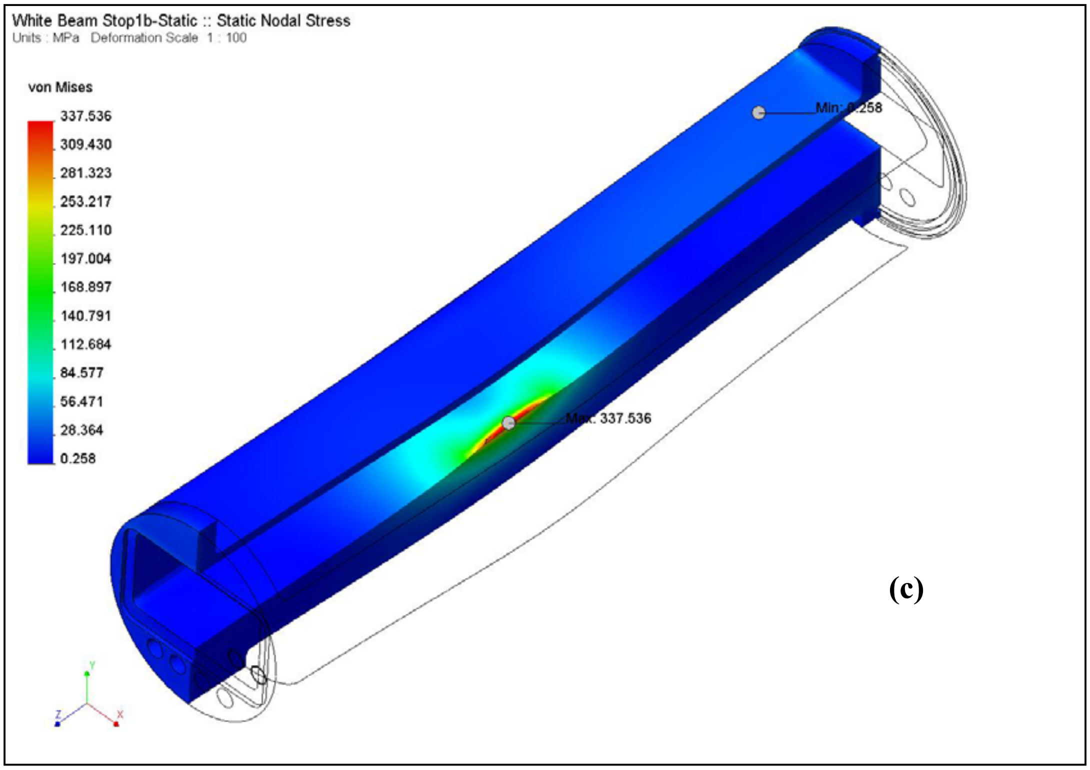


Figure 3.5 *Results of transient analysis for the total loss of coolant: (a) temperature as a function of time, (b) temperature at the onset of boiling, and (c) stresses at the onset of boiling.*

Loss of coolant in the two inner cooling channels represents the extreme case of a partial loss of coolant. The results of the analysis, as shown in figure 3.6, show that, once in steady state, the maximum temperature is 235°C, while the stresses reaches 315 Mpa. The temperature of the cooling channel walls is well below the boiling temperature. Although the partial loss of coolant does not lead to catastrophic failure, it should be noted that, when this happens, the most stressed parts of the mask body are exposed to plastic deformation, which may lead to fatigue failure.

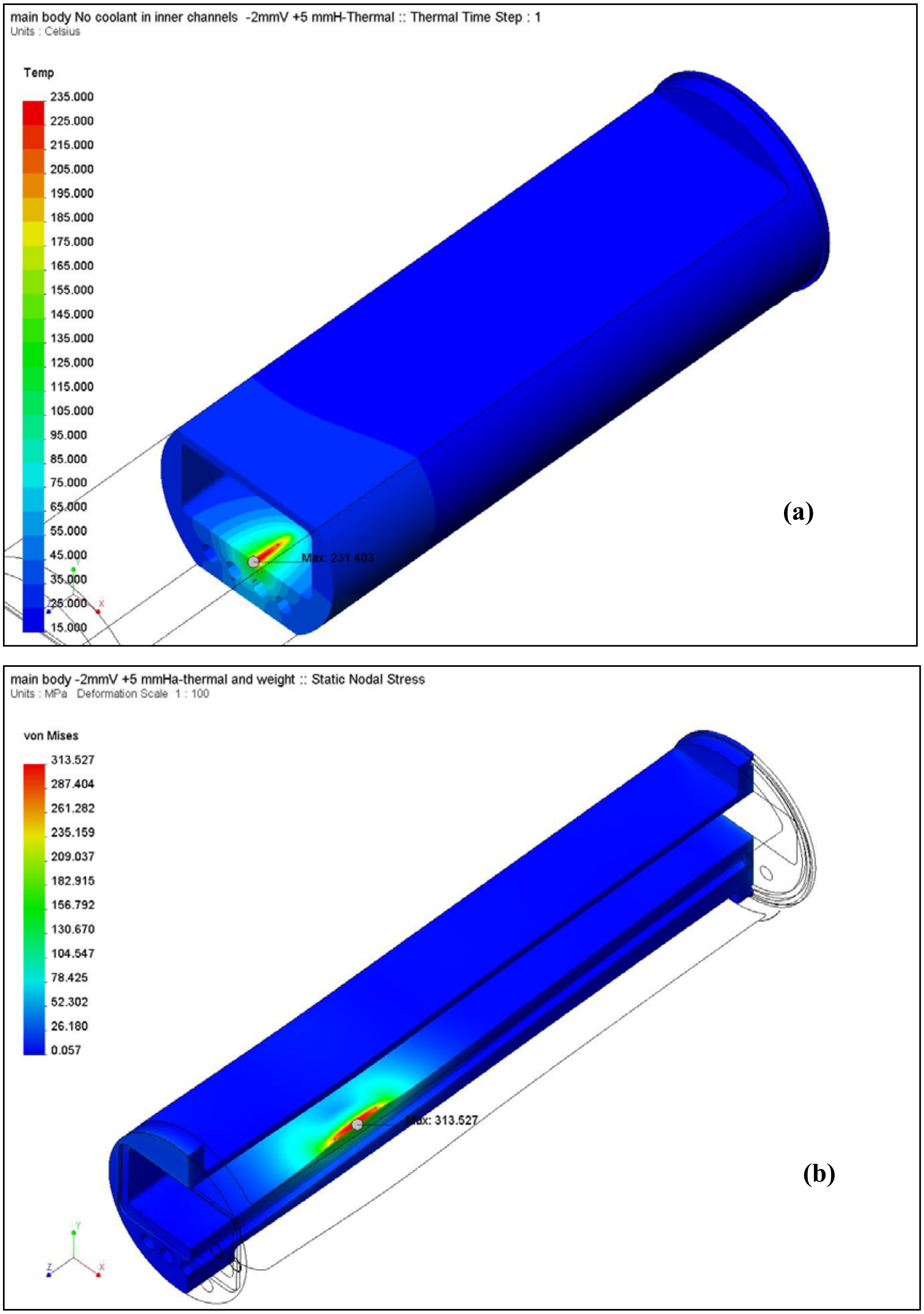


Figure 3.6 *The FEA results for the case of partial loss of coolant: (a) temperature distribution, and (b) stress distribution.*

3.3.5 MERIX High-Resolution Monochromator

The MERIX spectrometer requires medium-resolution (10^4-10^5) monochromatization over the energy range of 5-15 keV. Premonochromatization by a water-cooled double-crystal diamond (1 1 1) monochromator will produce an energy-dependent bandwidth that ranges from 0.3 eV at 5 keV to 1.2 eV at 15 keV (assuming full-source divergence on the monochromator). These bandwidths produced by the diamond (1 1 1) can be reduced efficiently by as much as 20% by reducing the incident white beam divergence on the monochromator. As there may be an interest in reducing the bandwidth to the 0.3 eV level at energies above 10 keV, an efficient solution is a double-crystal assembly (+a,-a) that uses an asymmetrically cut low-order reflection operating downstream of the diamond (1 1 1) premonochromator.

To extend the resolution to 10^5 efficiently, a 4-crystal medium-resolution monochromator will be used. Using a (+a,-a,+b,-b) crystal configuration and choosing the crystal reflections (e.g., a = b = silicon (8 0 0)) and the asymmetry-angles appropriately, it is possible to produce an efficient "constant-bandwidth" monochromator over an extended energy range. Specifically, a highly efficient 70-meV-bandwidth monochromator can be constructed of an "in-line" design (with zero-beam offset) that is continuously tunable from 5 keV to 12 keV. Figure 3.7 is a representation of the scheme to be used for the MERIX high resolution monochromator (HRM).

The implementation of these monochromator designs will require rotation stages with 0.5 microrad/step for the 0.3 eV bandwidth in the 10-15 keV energy range and two rotation stages with 0.1 microrad/step for the 100-meV-bandwidth monochromator. In addition, due to substantial absorption in air for x-rays below 10 keV, the 100-meV-bandwidth monochromator should be operated in a He/vacuum environment to preserve the photon flux.

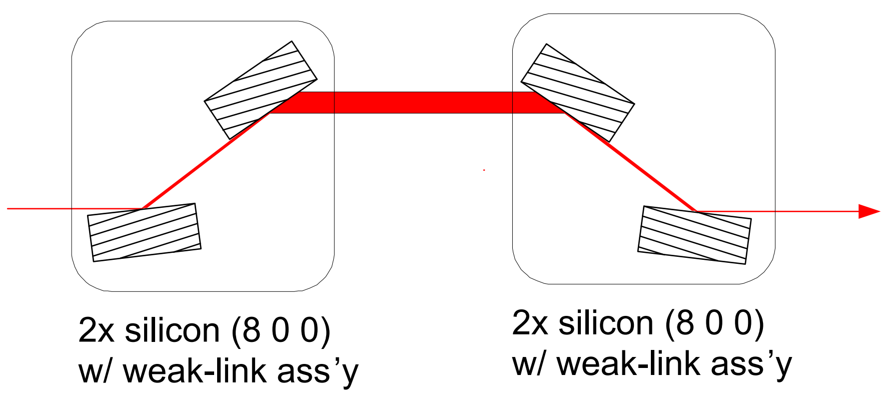


Figure 3.7 *Schematic representation of the four-crystal geometry for the MERIX HRM. Weak-link assembly (ass'y) refers to "artificially linked" crystals as described in D. Shu, T.S. Toellner, and E.E. Alp. AIP 521: Synchrotron Radiation Instrumentation: 11th US National Conference (2000) 219, Ed. P. Pianetta; and, D. Shu, T.S. Toellner, and E.E. Alp, U.S. patent granted No. 6,607,840 (2003).*

3.3.6 HERIX High-Resolution Monochromator

The HERIX spectrometer will operate at 25.701 keV, corresponding to the back-reflection energy of the silicon (13 13 13) lattice reflection. The HRM for the HERIX program will consist of six Bragg-diffracting silicon crystals arranged in a (+a,-a,-b,+b,+c,-c) configuration. The actual Miller indices and asymmetry angles for these reflections will be chosen to achieve a HRM design with optimal efficiency and an energy bandwidth of approximately 0.7 meV. The crystal reflections represented by "a" and "c" will be low-order silicon reflections (most likely the (2 2 0) reflection) operating at room temperature. The crystal reflection represented by "b" will be a very high order reflection (most likely the (18 12 6) reflection in silicon) that is cooled to silicon's zero-thermal-expansion-coefficient temperature of 123K. The two "b" reflections will be part of a monolithic channel-cut crystal, while all other reflections will be semi-independent crystal components. The exit beam will be parallel to the incident beam but offset vertically by not more than 5 cm. Figure 3.8 is a representation of the scheme to be used for the HERIX HRM.

Apart from the silicon crystals, the implementation of this configuration in a reliable and readily scannable design will require three high-resolution (nominally 25 nrad/step) rotation stages, two weak-link crystal assemblies, and one low-vibration cryostage. The rotation stages are commercially available, while the weak link crystal assemblies are designed and constructed locally. The low-vibration cryostage is currently under development.

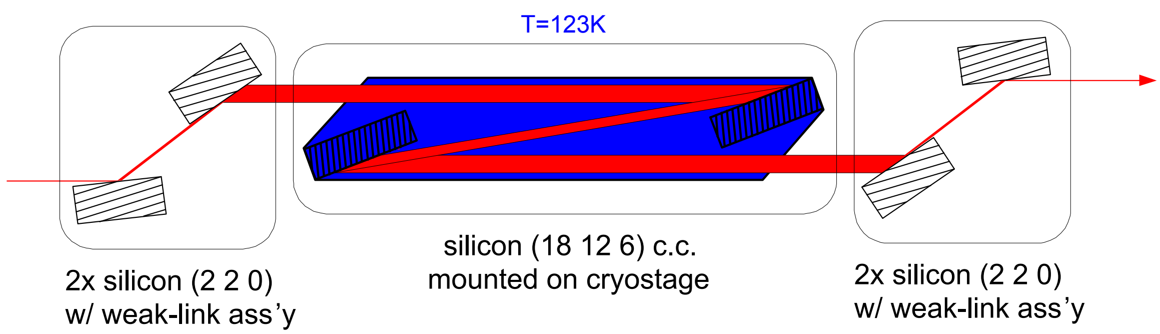


***Figure 3.8**: Schematic representation of the six-crystal geometry for the HERIX HRM.*

This HRM configuration has a number of advantages over previous multicrystal designs: single rotation-axis energy scanning, negligible temperature corrections to energy scale due to "b" operating at 123K, exit beam that is parallel to incident beam with only a 0-5 cm offset, and a spectral efficiency (for small collimated beams) that exceeds that of a single back-reflection (viz. silicon (13 13 13)) operating ideally at room temperature. This monochromator scheme has been designed by T. S. Toellner, and a similar six-reflection cryogenically cooled HRM is currently being built and will be installed and tested in 3-ID beamline at the APS during summer 2004.

3.3.7 MERIX Mirrors

A focus spot in the range of a few tens of micrometers is desirable for many applications. In addition to high-pressure experiments in diamond anvil cells, also many other scientific areas will benefit if a microfocus is routinely available. For that reason we chose KB mirror systems with adaptive bimorph bending technology. The mirrors for the MERIX spectrometer will operate around an incident angle of 4 mrad and will have either a Pd or Rh coating. Further details can be found in appendix D.

3.3.8 Monochromatic Shutter

The monochromatic shutter is the APS standard component P8-60 used in sector 3. Figure A.6 is the assembly drawing of the shutter. This shutter has a large vertical opening of 104 mm. This large opening will be used for the HERIX instrument when a different choice of resolution is preferred and the HRM is changed.

3.3.9 HERIX Mirrors

For the HERIX spectrometer, system very similar to the MERIX system was selected. Because of the higher energies up to 30 keV, a Pt and Rh coating and an incident angle of 2.3 mrad are necessary. Further details can be found in appendix D.

3.3.10 Vacuum Windows

For the most part, the beamline will use Be windows for vacuum barriers. The beamline has one Be window, which is exposed to white beam and is part of the front-end. The next Be window is located in the front of station B after the P5 shutter. The MERIX HRM is expected to be housed in a vacuum chamber. The K-B mirrors for the MERIX will be isolated from the beamline with two thin Be windows. The monochromatic shutter located behind the MERIX spectrometer is expected to share the same vacuum as the K-B mirrors in station C. Beryllium windows will be installed on either side, and the whole system is expected to be under vacuum pumped with ion pumps.

3.4 Instruments

3.4.1 MERIX Instrument

The MERIX spectrometer will be optimized for the study of moderate-energy excitations, with resolutions ultimately in the 0.05 – 0.2 eV range. Studies will be made both nonresonantly and resonantly (by tuning the incident energy near an absorption edge). With these resolutions, one is probing almost exclusively the dynamics of the electrons and the various electronic excitations. These excitations may be collective modes, such as plasmons, or single-particle-type excitations, such as particle-hole pair creation in a Fermi-liquid or excitations across a charge-transfer gap. The energy, dispersion and lifetime of such excitations play an enormously important role in determining the properties of essentially all materials of interest in solid-state physics.

The MERIX spectrometer will be designed to perform polarization-dependent measurements. This will be accomplished by having both vertical and horizontal diffraction capabilities with an 8-circle diffractometer. The expected sample-analyzer distance will be variable from 0.95 to 2 m. For the resonance experiments, a different analyzer will be required for each absorption edge. Existing technology utilizes various Si or Ge reflections and, by varying the Bragg angle of the analyzer, scans the energy transfer. In addition, we are presently pursuing the option of going closer to backscattering to take advantage of the increased angular acceptance of crystals at backscattering. We plan to have a suite of analyzers, made of various materials (such as Si, Ge, Al_2O_3, and $LiNbO_3$), so that many atomic resonance energies can be reached. In such cases, energy scans would then be performed by scanning the temperature of the analyzer and maintaining near backscattering conditions. Such methods allow scan ranges of 10-20 eV. A schematic of the spectrometer is shown in the figure 3.9 below.

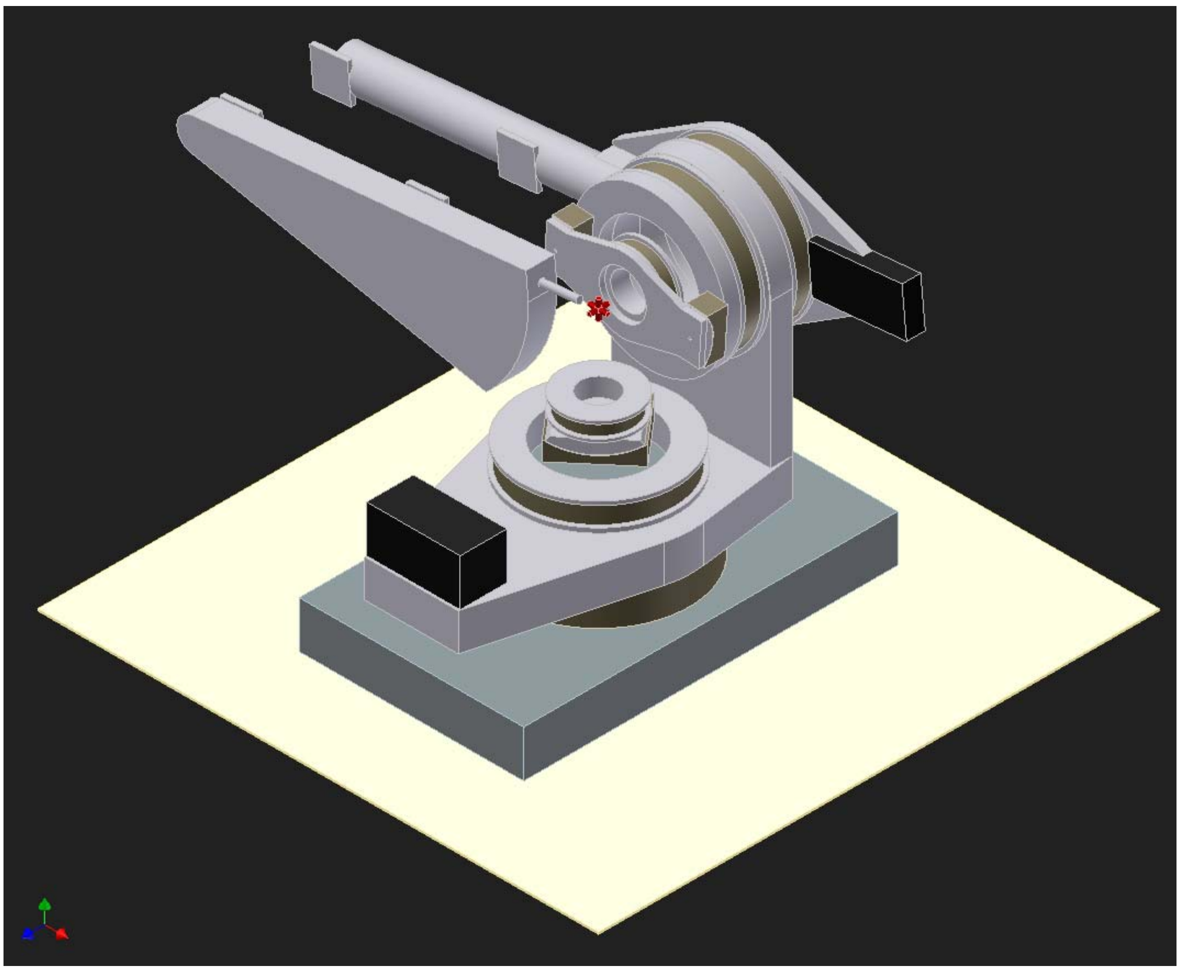


Figure 3.9. *View of the MERIX spectrometer in B station. The sample is located at the center of rotation. The spectrometer can be used in both horizontal and vertical planes.*

Presently we are planning on the following limits for the motor motions. Limits on two theta (tth) are due to the hutch shape and the upstream portions of the beamline.

Vertical Scattering

Motor	Range (degrees)
tth	-5 to 120
th	360
chi	-20 to 20
phi	360

Horizontal Scattering

Motor	Range (degrees)
tth	-5 to 120
th	360
chi	-20 to 20
phi	360

The height of the beam coming unto the spectrometer is determined by the monochromator setup, and the large vertical motion of the table is designed to allow for several different possibilities.

Table Motors

Motion	Range (mm)
x (towards/away from ring)	-25 to +25
y (vertical)	-45 to 95
z (along beam)	none

Energy analysis is provided by an analyzer crystal that is in a helium-filled flight path, which is used to reduce the attenuation from the air. Below are the present motion limits based on our flight-path design.

Analyzer motions

Motor	Motion (degrees or m)
tth @2 m	0 to 13
tth @ 1 m	0 to 30
th	-5 to 35
chi	-5 to 5
trans (distance from sample)	0.95 to 2.05

3.4.2 HERIX Instrument

When fully implemented, the HERIX spectrometer is expected to outperform all existing inelastic spectrometers in terms of energy resolution, flux on the sample, number of analyzers, and beam size on the sample. The design parameters are:

Energy resolution:	0.8 – 2 meV
Working energies:	25.7 keV – 21.6 keV
Number of analyzers:	9 (expandable to 16~18)
Momentum transfer range:	0.5 nm^{-1} – 78 nm^{-1}
Maximum scattering angle:	35°

Distance sample-analyzers: 9 m
Width of vacuum chamber at downstream end: 1.6 m (10° horizontal opening angle)

At the sample space, there will be a multipurpose goniometer setup that allows precise positioning of even heavy-sample environments like cryostats and ovens. Moreover, the sample goniometer table can be removed completely and enable large setups like laser-melting facilities, etc. (see figures 3.10 and 3.11).

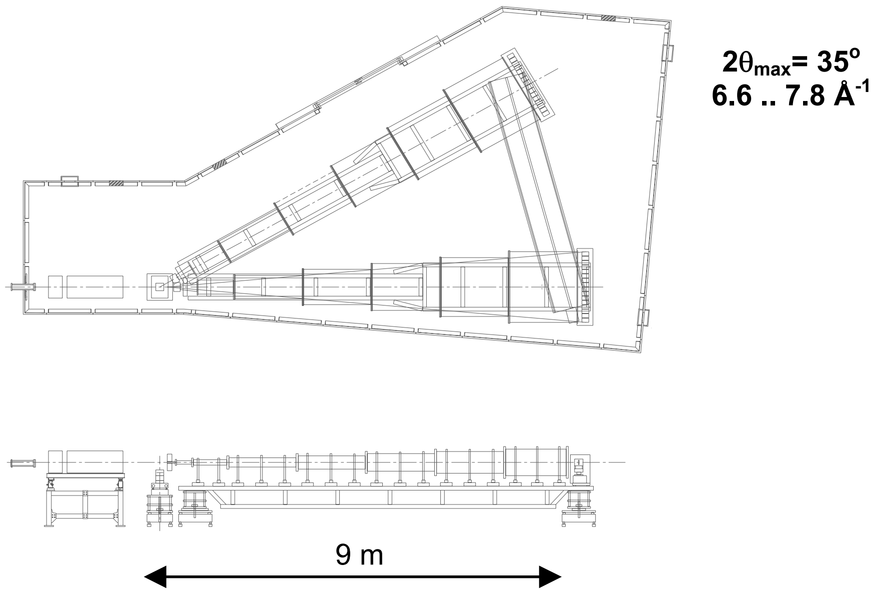


Figure 3.10 *View of the HERIX spectrometer in C station. The large vacuum vessel is the flight path between the detector and nine analyzers that are used simultaneously. The 9-m-long arm holding the vacuum vessel and the analyzers can rotate around the sample position by 35 degrees.*

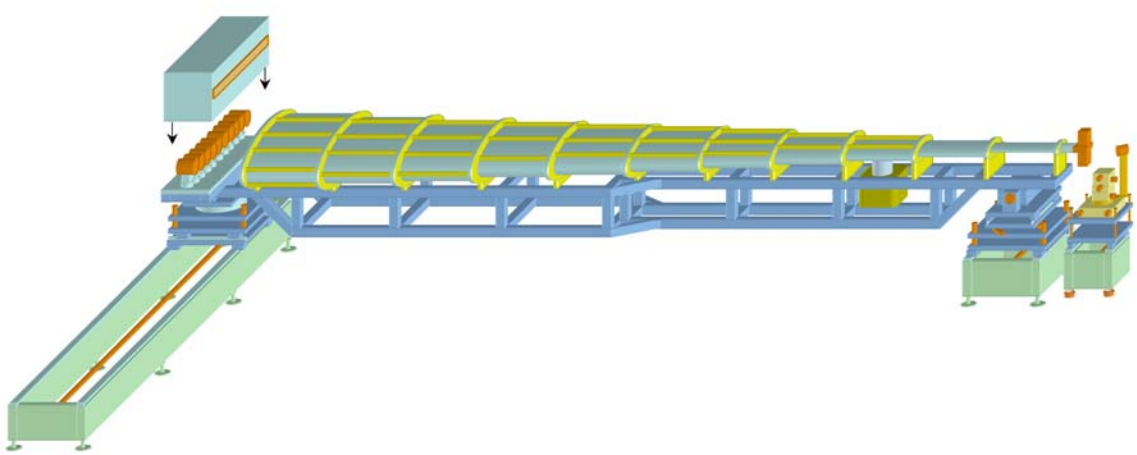


Figure 3.11 *Schematic design of the HERIX analyzer setup with the sample stage on the right side.*

The vacuum chamber is designed for nine analyzers in the scattering plane, which will offer the same geometry and thus the best possible energy resolution for all analyzers. Future upgrades to 16 and more analyzers are possible; however, they will require a further integration of the detector and the analyzer design.

3.4.2.1 Analyzers

Most of the R&D was or is currently done at the 2 meV inelastic spectrometer at sector 3. The feasibility of reaching 1 meV overall energy resolution was demonstrated in 2002 (see figure 3.12 left) on the 6-m-long analyzer arm. As calculations of the resolution function show (figure 3.10 right), the 9 m analyzer arm at HERIX should allow sub-meV resolution without losing intensity, by slitting down the beam at the detector as was done in the sector 3 test experiments. All critical parts of the analyzer fabrication (dicing, etching, bonding) are done at the APS. For the case of up to nine analyzers, no major changes in the analyzer design are necessary. The temperature stability and thermal gradient should be improved from currently 10mK to 5mK. Also an improvement of the typical figure error of currently 25 microradian would improve the efficiency, and recent tests with anodic bonding look very promising. We plan to optimize the analyzers during 2004 with further tests and commissioning experiments at sector 3. For future upgrades with more than nine analyzers, a more compact design for analyzers is needed with either a simplified bending mechanism or a fixed bending radius.

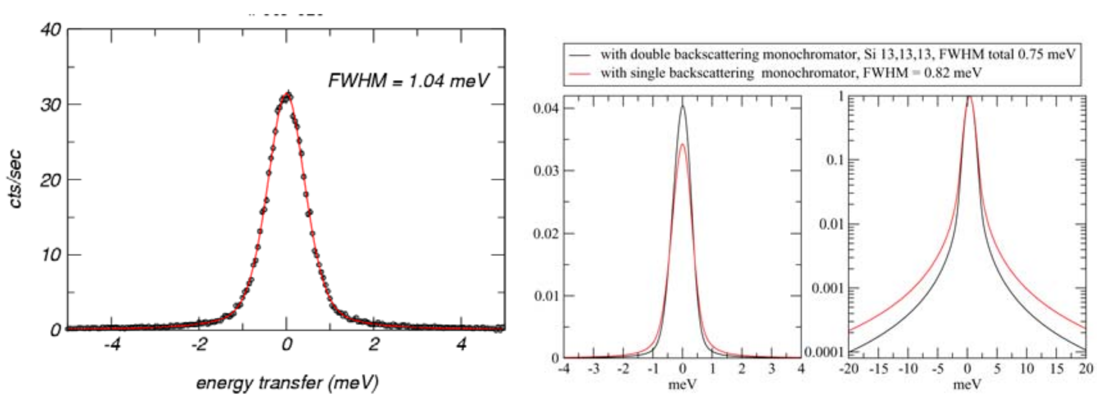


Figure 3.12 *Resolution function measured at 3ID with a 6-m-long analyzer setup (left). Calculated resolution function for the HERIX spectrometer (right).*

3.4.2.2 Detectors

The current detector at sector 3 is a four-element CdTe detector from AMPTEK with 6 mm center-to-center distance between elements (figure 3.13). This detector was tested at sector 3 and seems to work fine even though some ultrasound-bonded wires broke during the first cooling cycles. We expect that these minor problems can be fixed soon. The HERIX requires a nine-element detector, which will be a combination of a four- and a five-element detector above and below the scattering plane. The spacing of the CdTe elements and the electronics are identical to the existing four-element detector, so that there should be no further problems that would delay the commissioning phase. By having two independent detectors the reliability is also enhanced, since one detector can still be used if the other one fails.

A future upgrade to, e.g., 16-18 analyzers would require the distance between elements to be changed from 6 to 3 mm. According to information from AMPTEK, this is feasible, however it, would require some research and development (R&D) on their part.

Figure 3.13 *Four element CdTe detector used in sector 3. For HERIX, a four-element and a five-element detector will be used in tandem.*

3.4.2.3 Vacuum chamber for the multianalyzers setup

The vacuum chamber and the approx. 9-m-long supporting arm are considerably heavier than the setup at sector 3. Currently the design of the vacuum chamber and the arm have been modeled with FEA (see figure 3.14). In early 2004, the design of these components will be finalized.

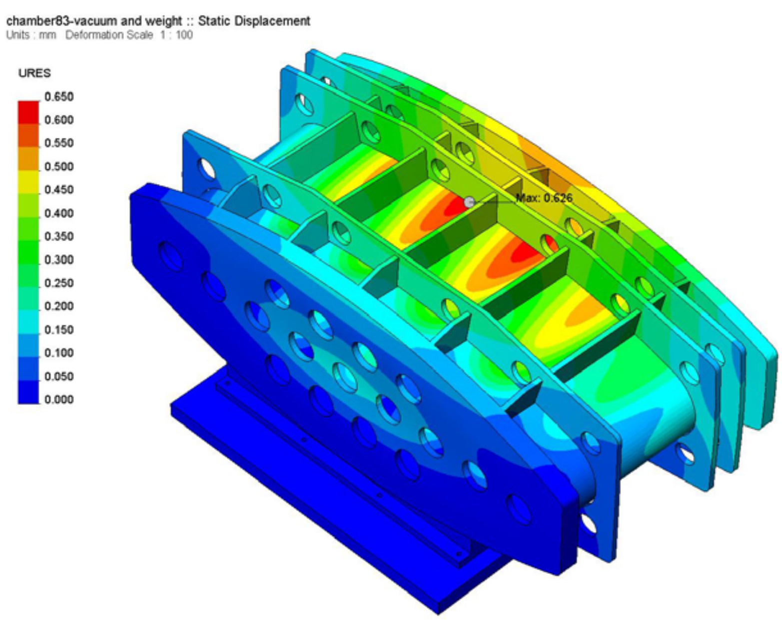


Figure 3.14 *Finite element analysis for a possible design of the last section of the vacuum chamber shown in fig. 3.11.*

4 Preliminary Safety Analysis

The beamline design is very simple. There will be no white beam operation. All operation will be with monochromatic beam in stations B and C. There are no shielded beam transports as all three stations are attached to each other.

4.1 Shielding Design

The beamline shielding conforms to all APS standards. The stations have been designed after consultation with the APS radiation scientist. The beamline has three stations continuously. Figure A.7 shows the layout of the stations as provided to the station-shielding vendor. All drawings are part of the APS Document Control center (DCC). Of the three stations, only the FOE is a white beam station. We expect this beamline to operate with as many as three 3.0 cm period devices and a 1.45 cm period SCU. As such, based on the recommendation of the APS radiation physicist, the shielding of the FOE has been increased. (Even though the calculations by APS radiation physicist show the current requirements are adequate.) The other two stations are monochromatic and conform to APS standards for monochromatic stations.

The beamline has no exposed beam transports due to the nature of the beamline design. In addition there are no shielded transport as there are no pass-through modes. All beamline components are located inside one of the three stations. The two shutters are located in stations A and B, respectively. Figures A.8 and A.9 are the bremsstrahlung ray tracings and figures A.10 and A.11 are the horizontal and vertical synchrotron radiation optical-aperture ray tracings.

4.2 Personnel Safety System

The Personnel Safety System (PSS) will be designed and installed by the APS. The logic for this beamline is straightforward. There are three stations and each station has a shutter associated with it. Access to station A is controlled by the front-end shutter inside the shield wall. Station A is a white beam station and has three doors. Figure A.12 shows the layout of the various PSS components, to be installed by the shielding-enclosures vendor. Stations B and C are monochromatic, and their PSS layouts are shown in figures A.13 and A.14, respectively. The white beam stop in the rear of station A consists of a fixed photon stop mask and a fixed tungsten bremsstrahlung collimator inside a vacuum system. All white beam is stopped here. These are part of the P5-80 integral shutter. In addition this shutter has two monochromatic shutters to stop monochromatic beam from entering into station B. The white beam photon stop will be interlocked to the PSS via the water flow and the differential pressure. The monochromatic shutters will be interlocked to the PSS to provide access to station B. At the back of station B is a P8-60 monochromatic shutter to stop the beam from entering station C.

The IXS-CDT has reached an understanding with the ASD Safety Interlocks (SI) Group to use this beamline as a test bed for the PSS generation-III system. The IXS-CDT will provide access to the stations for SI Group personnel as soon as the construction of the stations are complete. In addition SI Group personnel will have numerous months of testing and fine-tweaking time prior to IXS-CDT starting serious commissioning of the beamline.

The beamline expects the main PSS controls to be EPICS based. However, as a backup, we expect the SI Group to provide one touch screen to control the station shutter located adjacent to the station C doors.

4.3 Equipment Protection System

The beamline equipment protection system (EPS) will be designed by the SI Group of ASD based on IXS-CDT specifications. The beamline EPS is expected to be very simple. The EPS system will be based on programmable logic controllers (PLC) and will be used to monitor the water flow on all non-critical white beam components. In addition the system will be used to operate the vacuum valves. All ion pumps and vacuum gauges will be interlocked with the gate valves via the PLC. In addition temperatures of some of the beamline components will be monitored via the PLC. The EPS PLC will be interfaced into EPICS. All controls and monitoring of the EPS system can be performed either via a touch system or the EPICS graphical user interface (GUI) screens.

5 Cost and Schedule

The IXS-CDT has a commitment from the DOE of $5M over a period of five years starting from 2002. The fiscal year for this funding starts in February, and the last installment of $1M from DOE is expected in February 2006. These funds are provided to Western Michigan University. The IXS-CDT also has a commitment from NSF for $900,000 over three years starting in February 2002 to be used towards the HERIX instrumentation. In addition certain member institutions of the CDT have committed $550,000. These funds are handled by SUNY at Stony Brook. Finally, the APS will be providing significant assistance in the design, procurement and operational aspects of the CDT through the assignment of APS personnel to IXS-CDT responsibilities, including front-end, specialized undulators, the implementation of the extended straight section, and operational issues.

Appendix E is a comprehensive WBS with a detailed cost and schedule for the whole beamline from construction through the start of commissioning. The operation of the beamline will be handled by the APS.

6 Additional Operational Requirements

The beamline at this time has no laboratory office module (LOM). The beamline will have a control room area adjacent to the stations as shown in figure A.1 The control room area construction is coordinated with the APS conventional facilities and will be awarded as contract through the APS. The control room area will have fire protection in the form of smoke detectors and sprinklers and will conform to all ANL requirements. The control room area will also be tied to the building HVAC system.

7 R & D Plans

The current IXS-CDT proposal requires the following research and engineering development programs for IXS-CDT plans to reach their full potential:

- Extension of the straight section of the APS storage ring:

Lattice simulation studies need to be done, accompanied by machine studies, in order to implement a longer straight section that is consistent with APS long-term storage ring upgrade goals, such as lower emittance and higher stored currents.

- Undulator vacuum chambers for longer straight sections:

Current vacuum chambers are designed to accommodate 5-m-long undulators. A new design is needed to accommodate longer straight sections.

- Superconducting undulator:

The HERIX experiments require an undulator that delivers ~25 keV in the first harmonic. To achieve this with a K of around 1 requires a device, that has a magnetic field of about 0.8 Tesla at 0.8 cm gap and 1.45 cm period. APS has undertaken the required R&D and is working to deliver a prototype SCU for IXS-CDT.

- Front end with high-heat-load handling capacity:

While the anticipated heat load at 100 mA seems to be within the limits of the current safe-operation envelope, it was necessary for the APS to look into modifications in the current front-end design to accommodate higher stored current in the storage ring that may take effect in the near future. This work has now been completed, and the design of the front-end is at the review stage at the time of the writing of this report.

- Cryogenically cooled high-resolution monochromator for HERIX:

To improve the performance of the HERIX monochromator, the sector 3 instrumentation program must include the development of a cryogenically cooled monochromator. We need a turn-key system ready for a user program. The prototyping and specifications for a vendor-built system, procurement, installation and commissioning are expected to be performed by XOR personnel.

- Dynamically bent analyzer for HERIX and MERIX:

The possibility of using either a 2 or 9 m analyzer requires the availability of analyzer-mounting mechanisms capable of bending to different radii. The current developments at sector 3 of XOR are encouraging, and, therefore, we anticipate that sector 3 staff will develop mechanical parts for the analyzers for HERIX and MERIX instruments.

- Sapphire analyzers for MERIX:

In order to benefit from increased angular acceptance near backscattering angles, we plan to use a number of different analyzers, in particular sapphire, which will be developed by XOR. Many of the manufacturing issues related to sapphire-analyzer development have been addressed, and potential solutions have been found. Currently, a full time graduate student is working on this issue.

Appendix A. Beamline Layout and Ray Diagrams

Figure A.1 Sector layout.

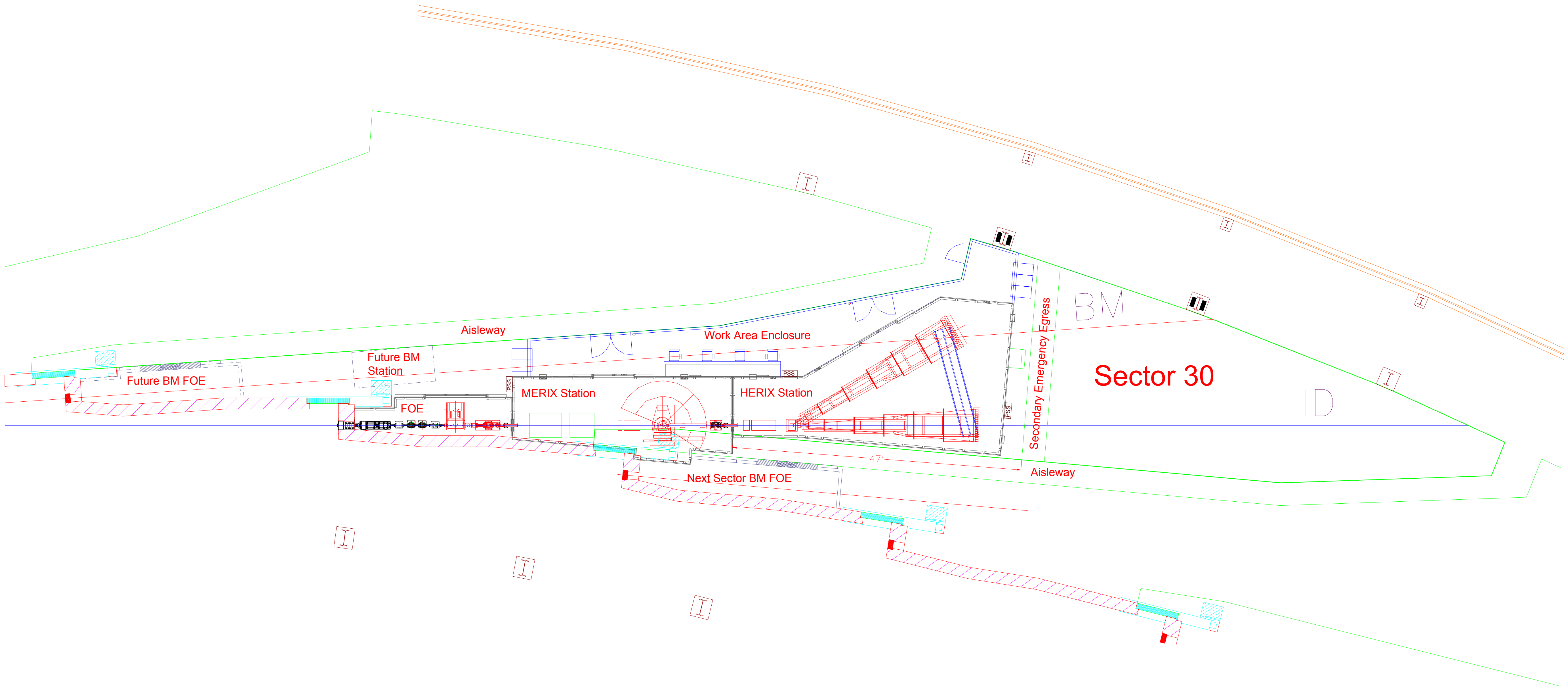


Figure A.2 Beamline layout with plan & elevation view.

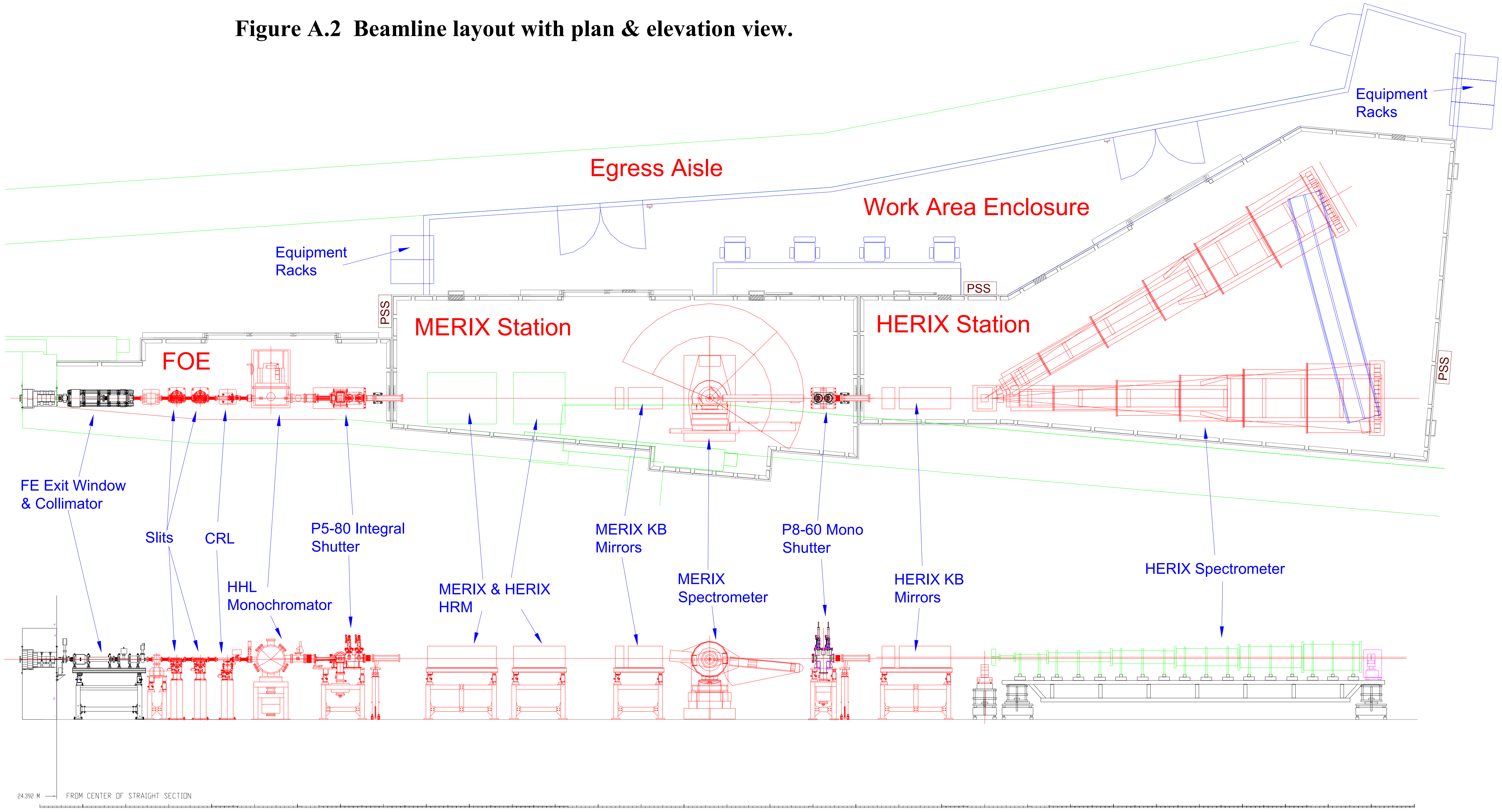


Figure A. 3 Beamline utility layouts.

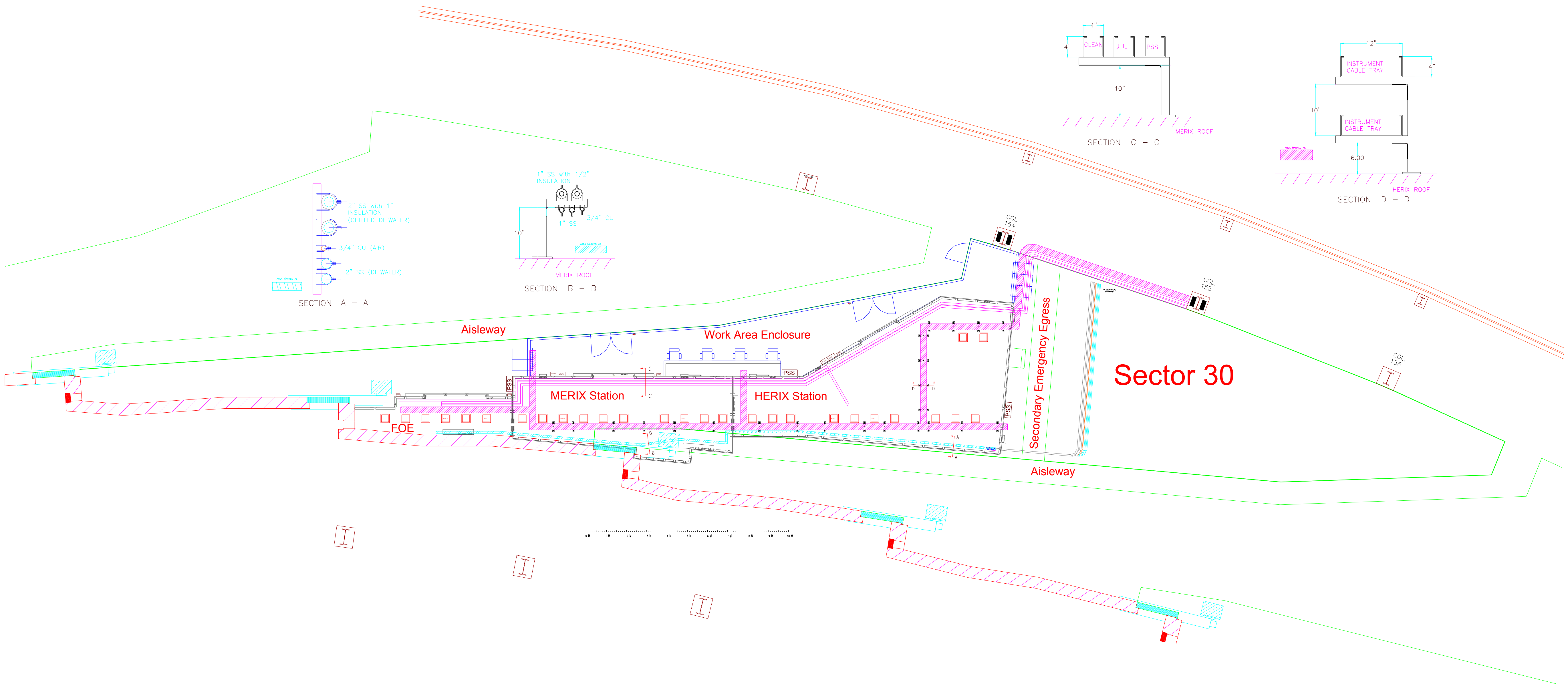


Figure A.4 White beam slits and compound refractive lens assembly.

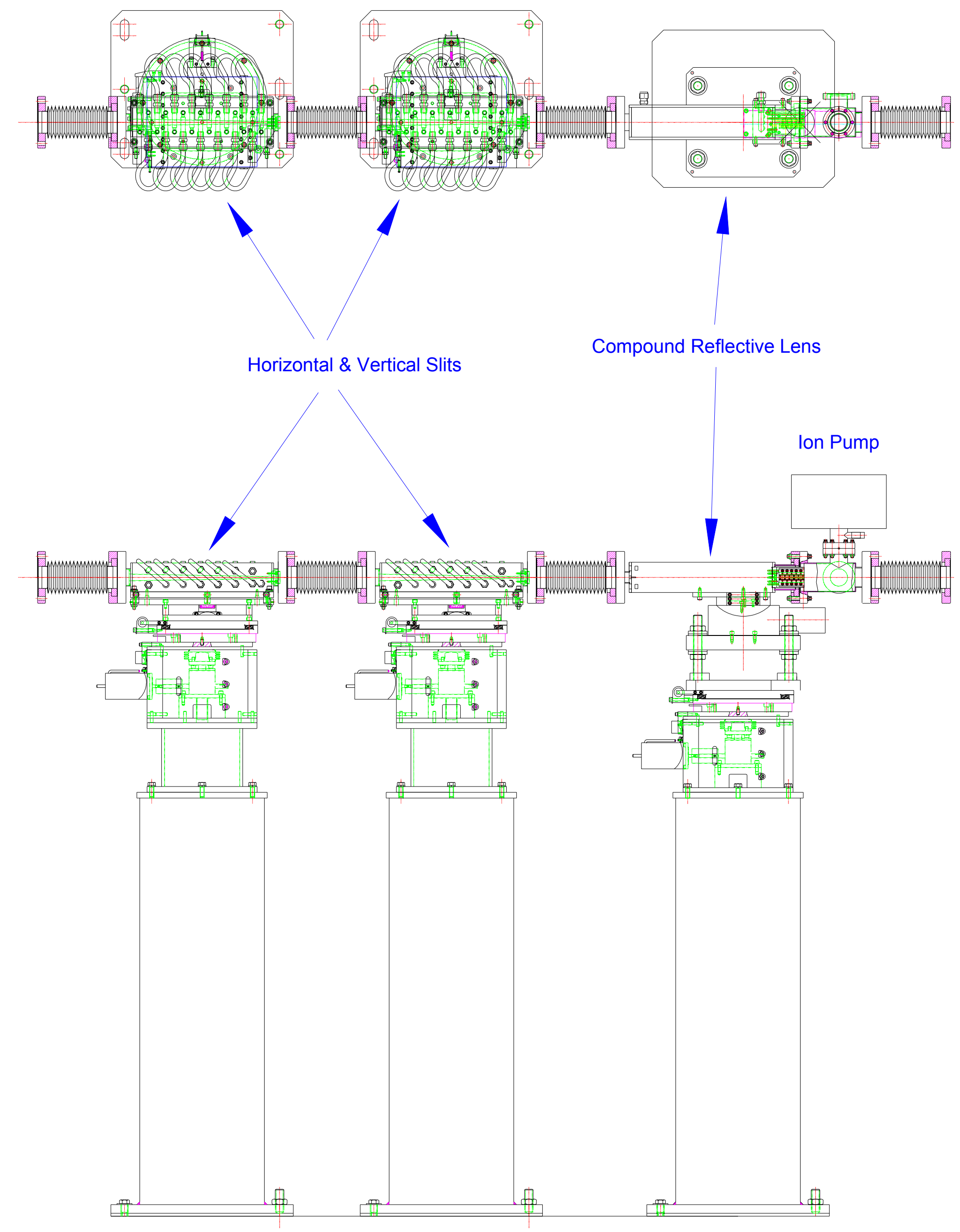


Figure A.5 Integral shutter (P5-80) assembly.

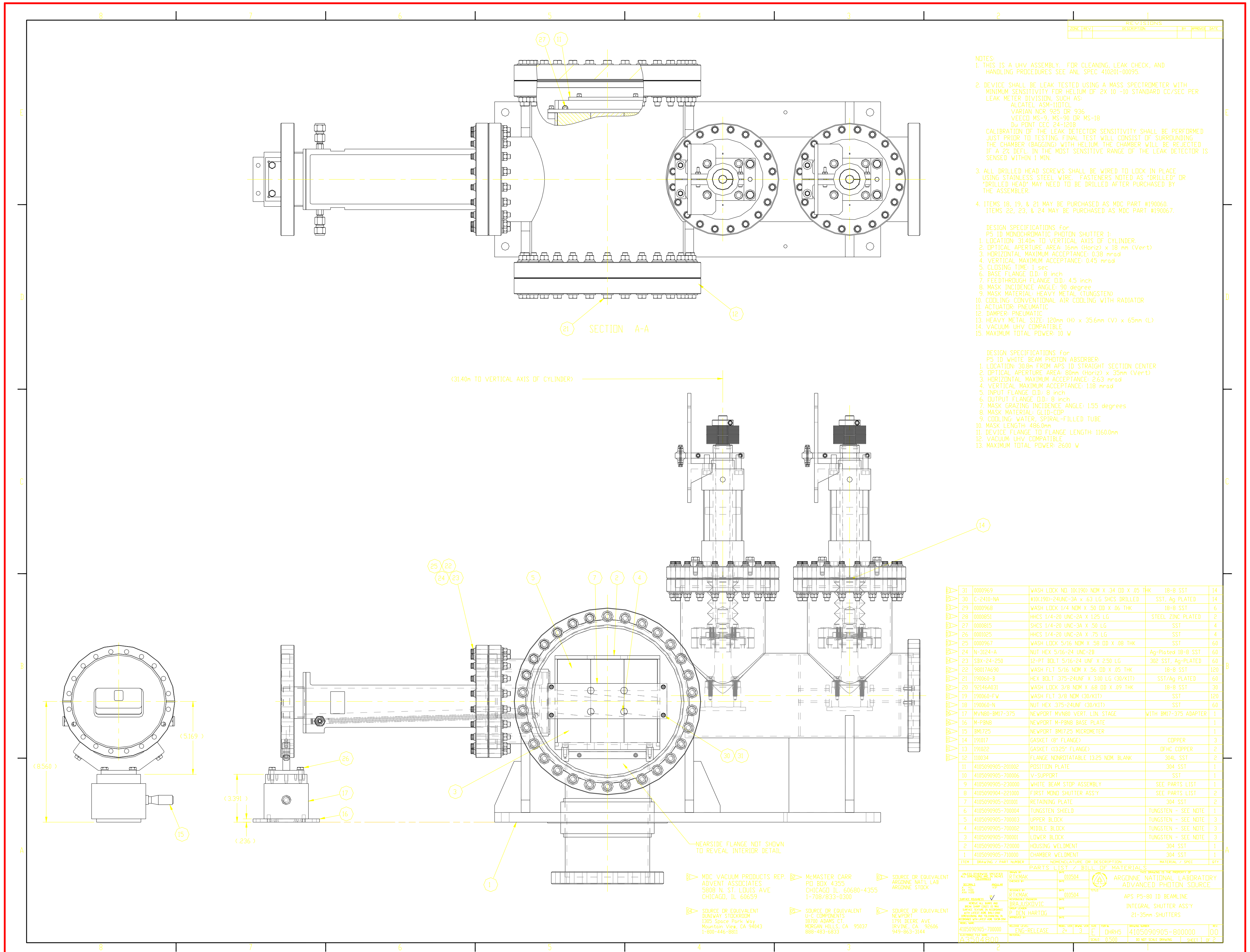


Figure A.6 Monochromatic shutter (P8-60) assembly.

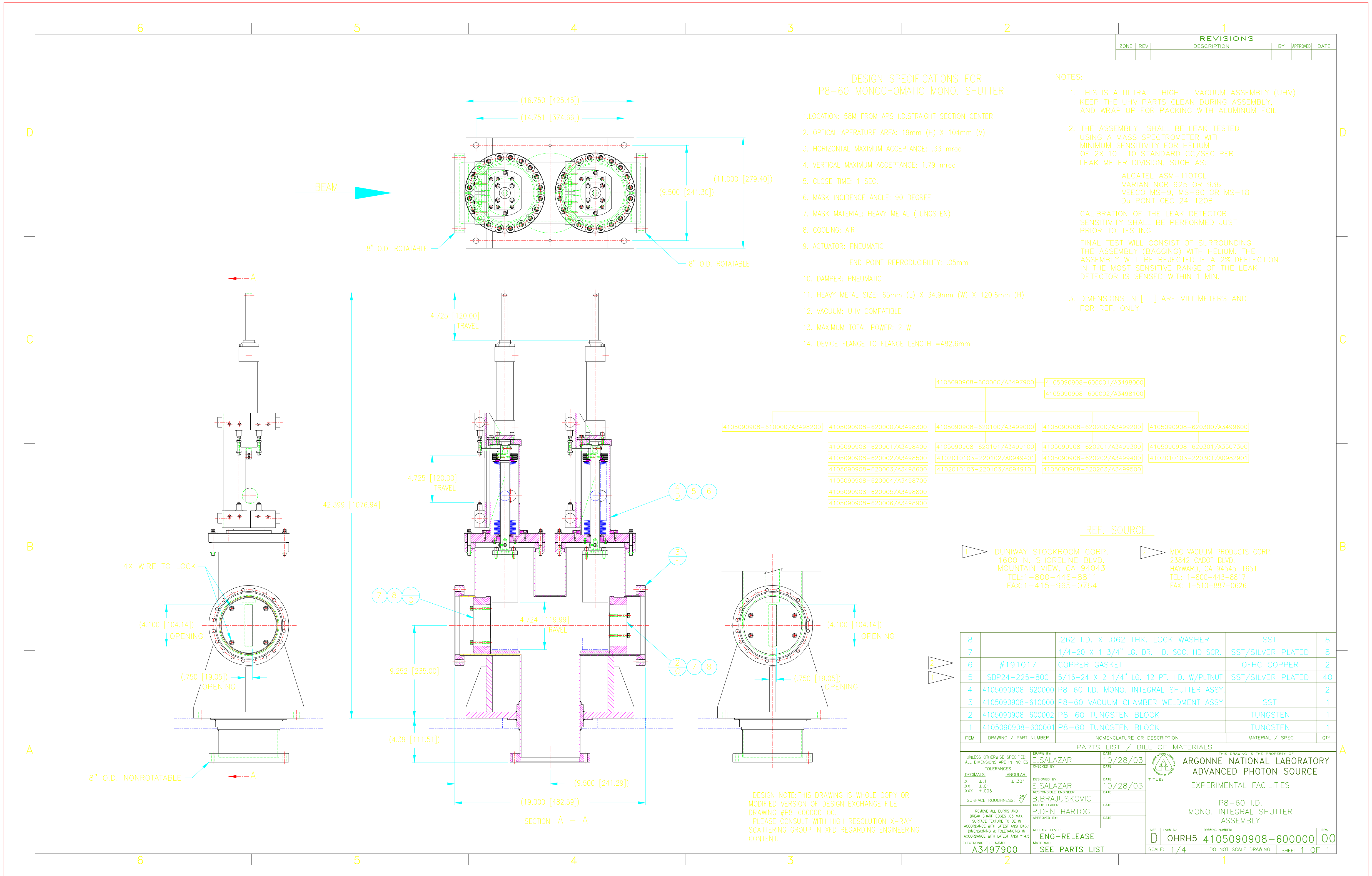


Figure A.7 Beamline shielding enclosure layout.

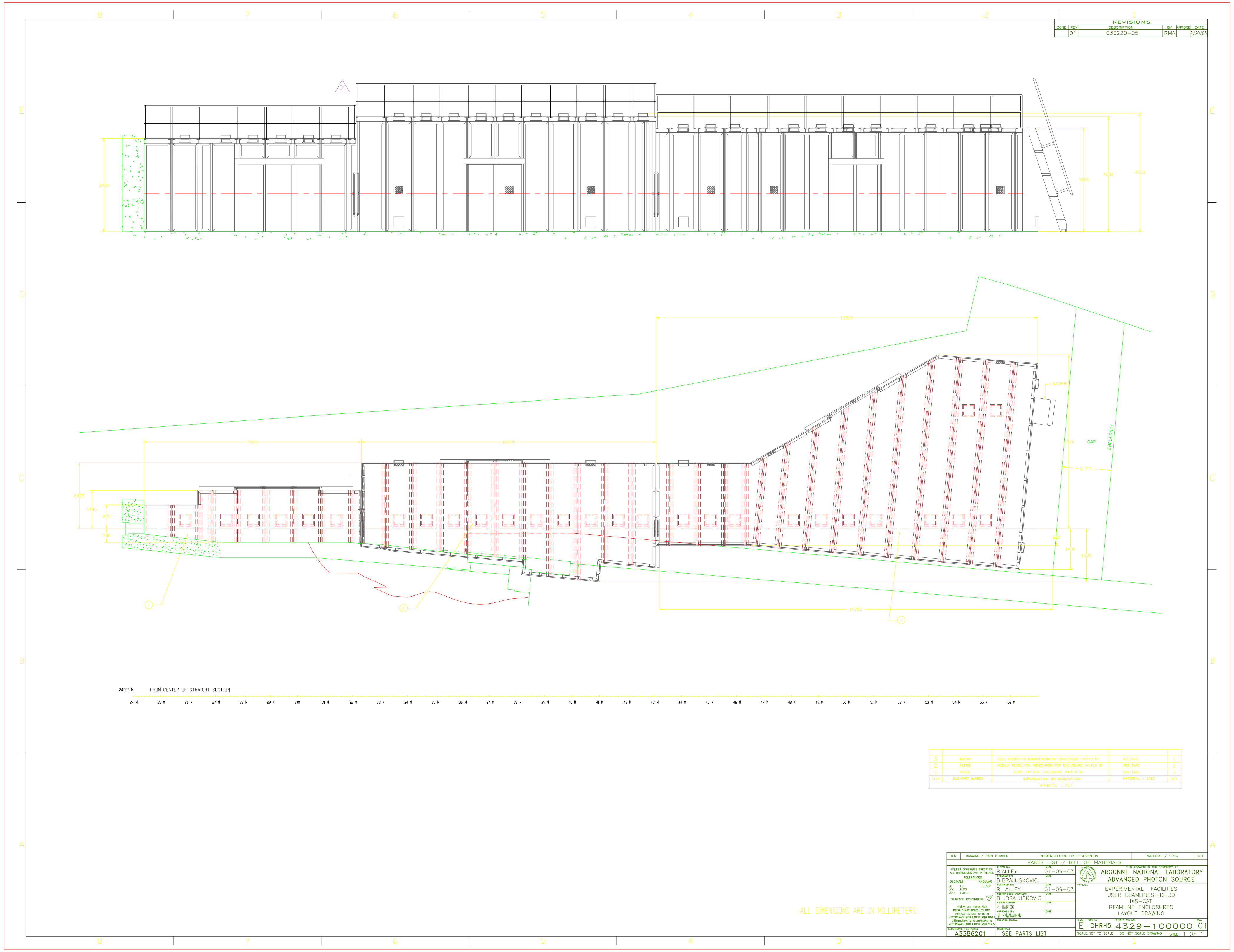


Figure A.8 Horizontal bremsstrahlung ray tracings.

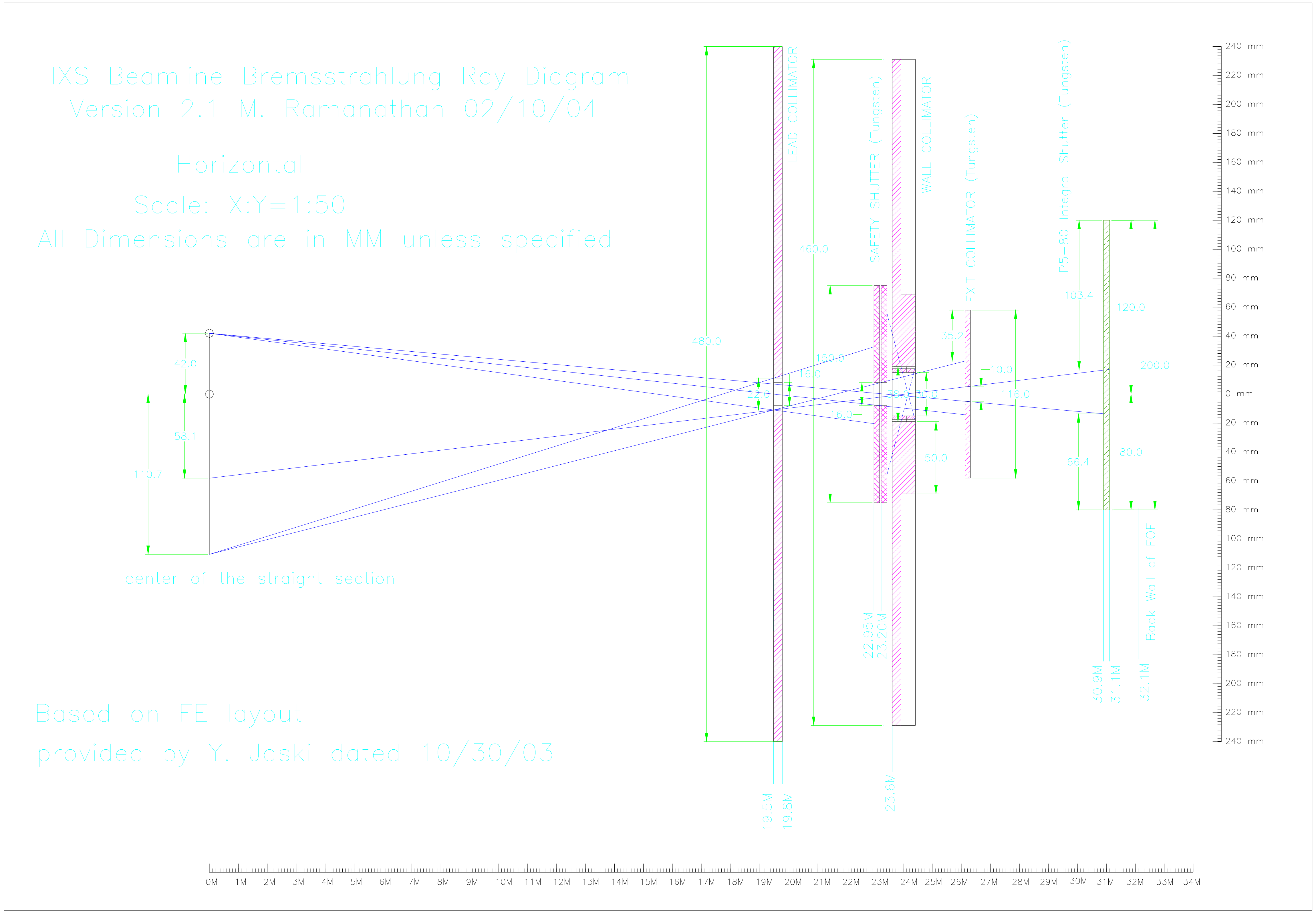


Figure A.9 Vertical bremsstrahlung ray tracings.

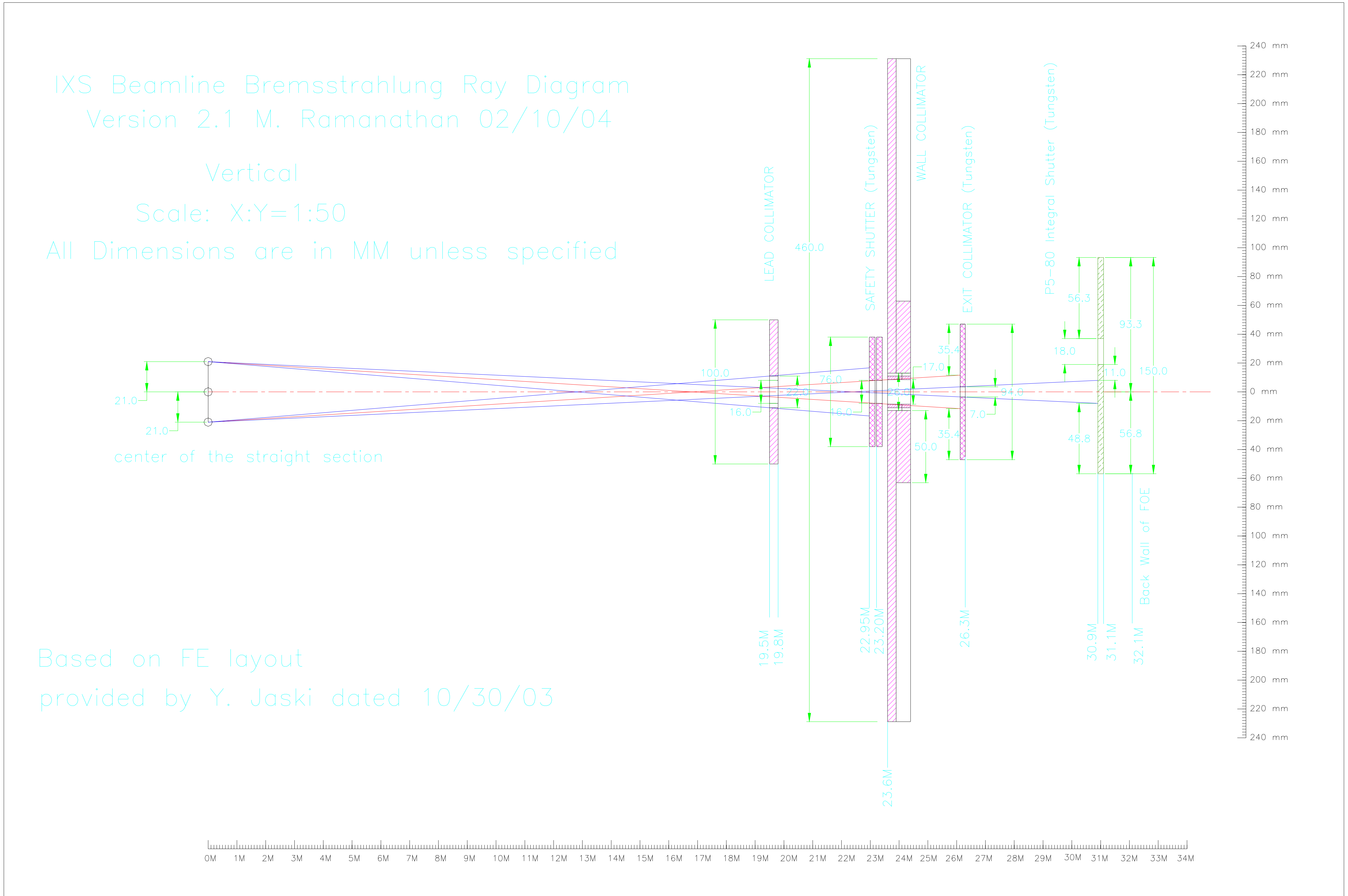


Figure A.10 Horizontal synchrotron radiation optical aperture ray tracings.

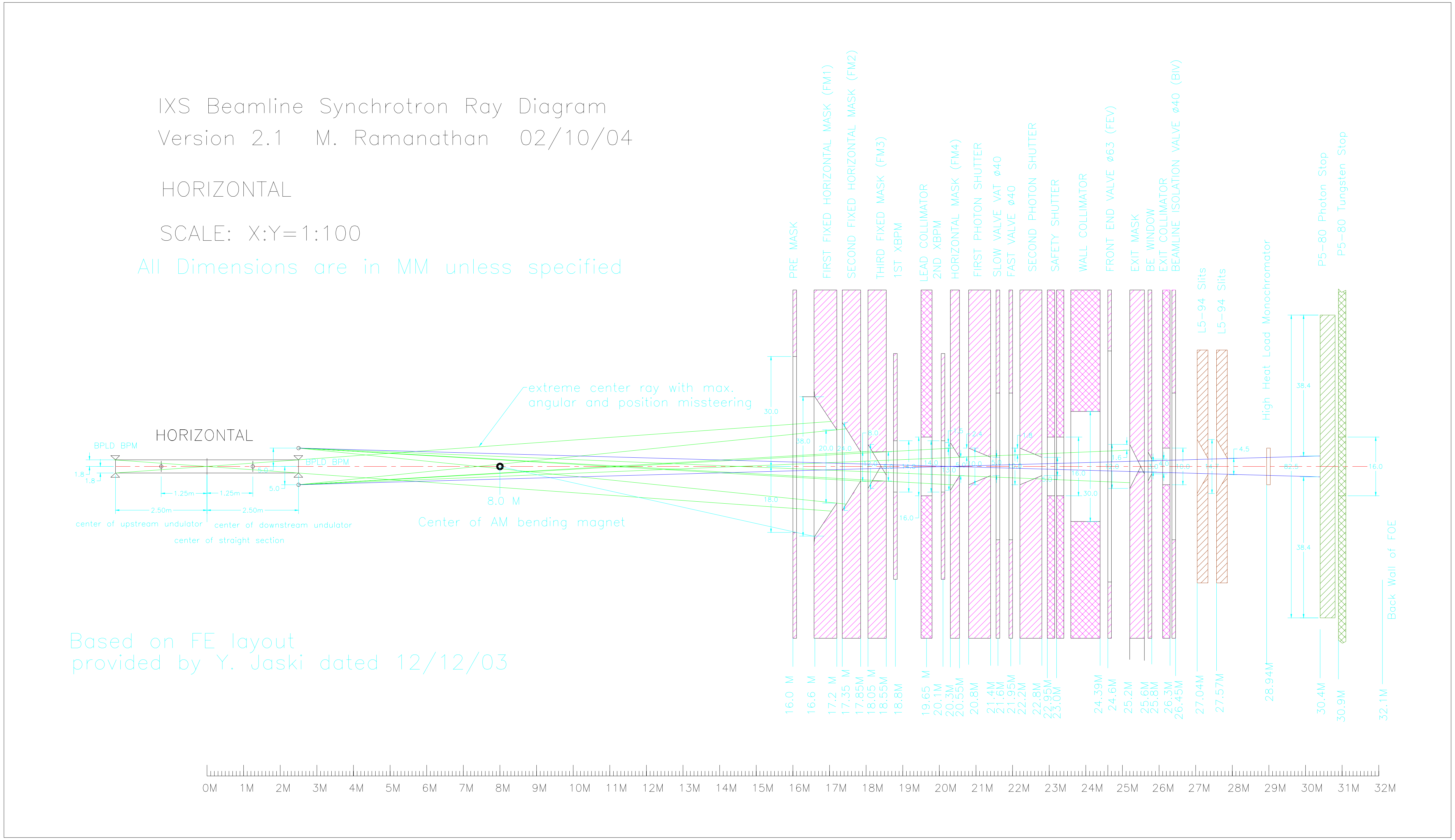


Figure A.11. Vertical synchrotron radiation optical aperture ray tracings.

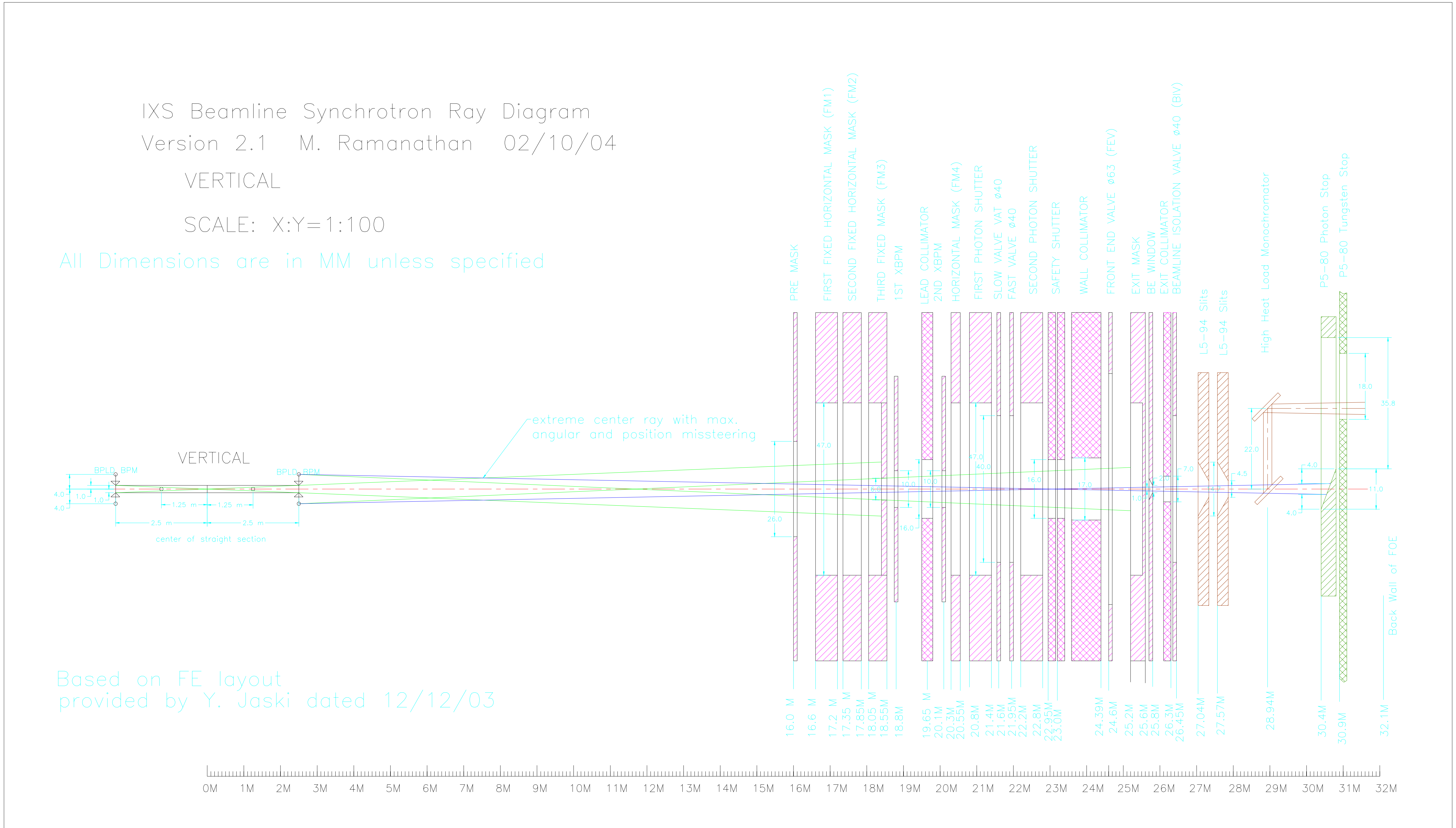


Figure A.12. Personnel safety system layout for station A.

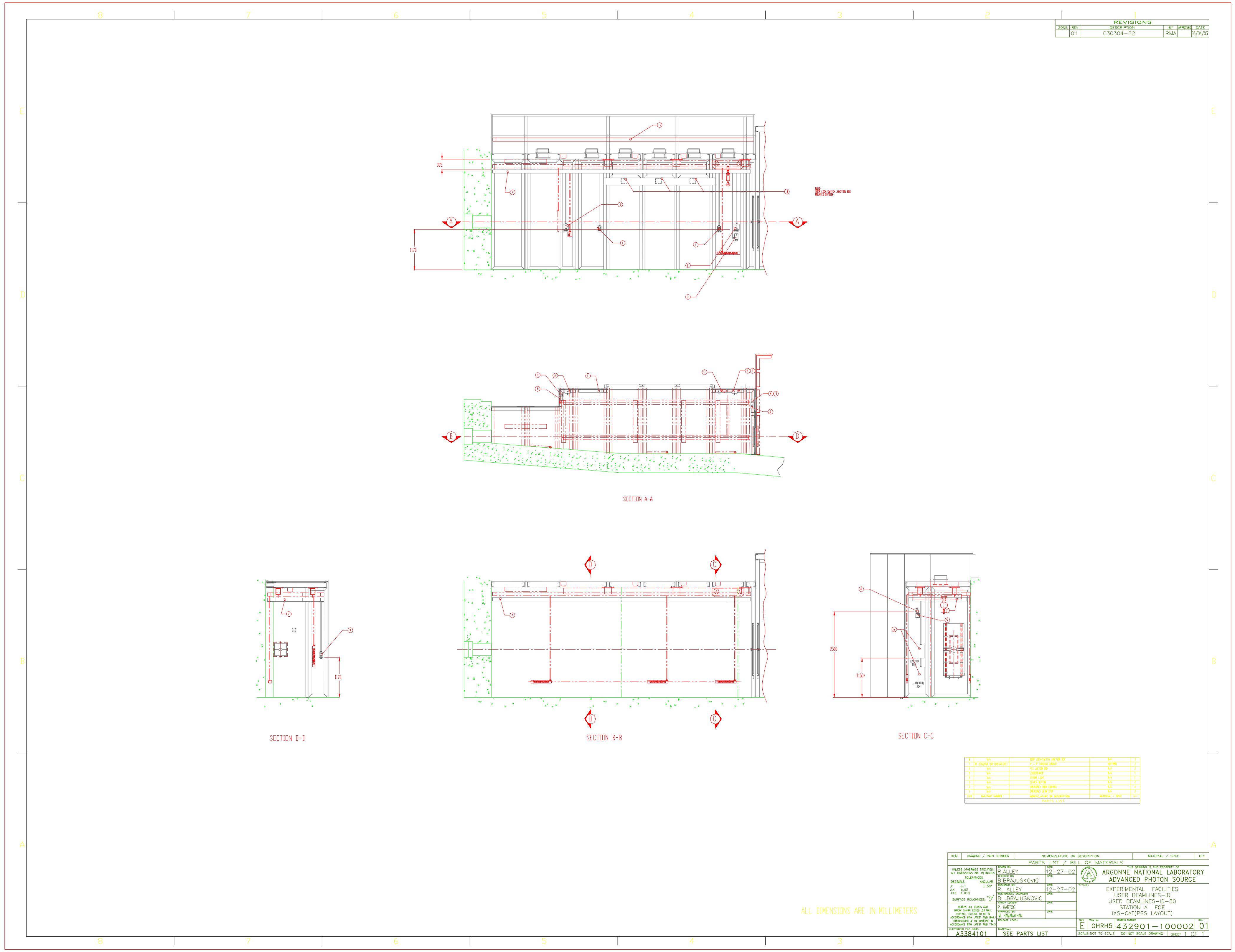


Figure A.13 Personnel safety system layout for station B.

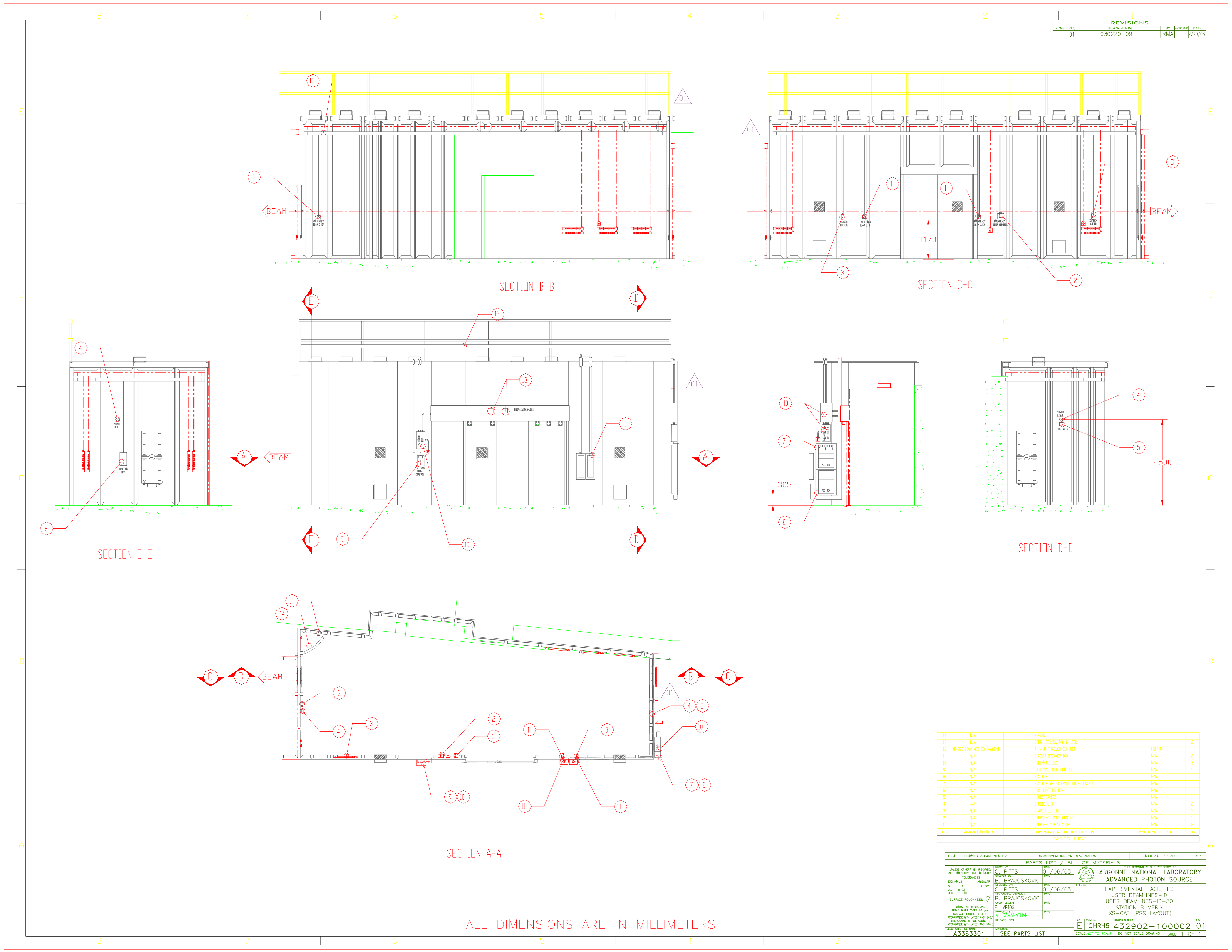
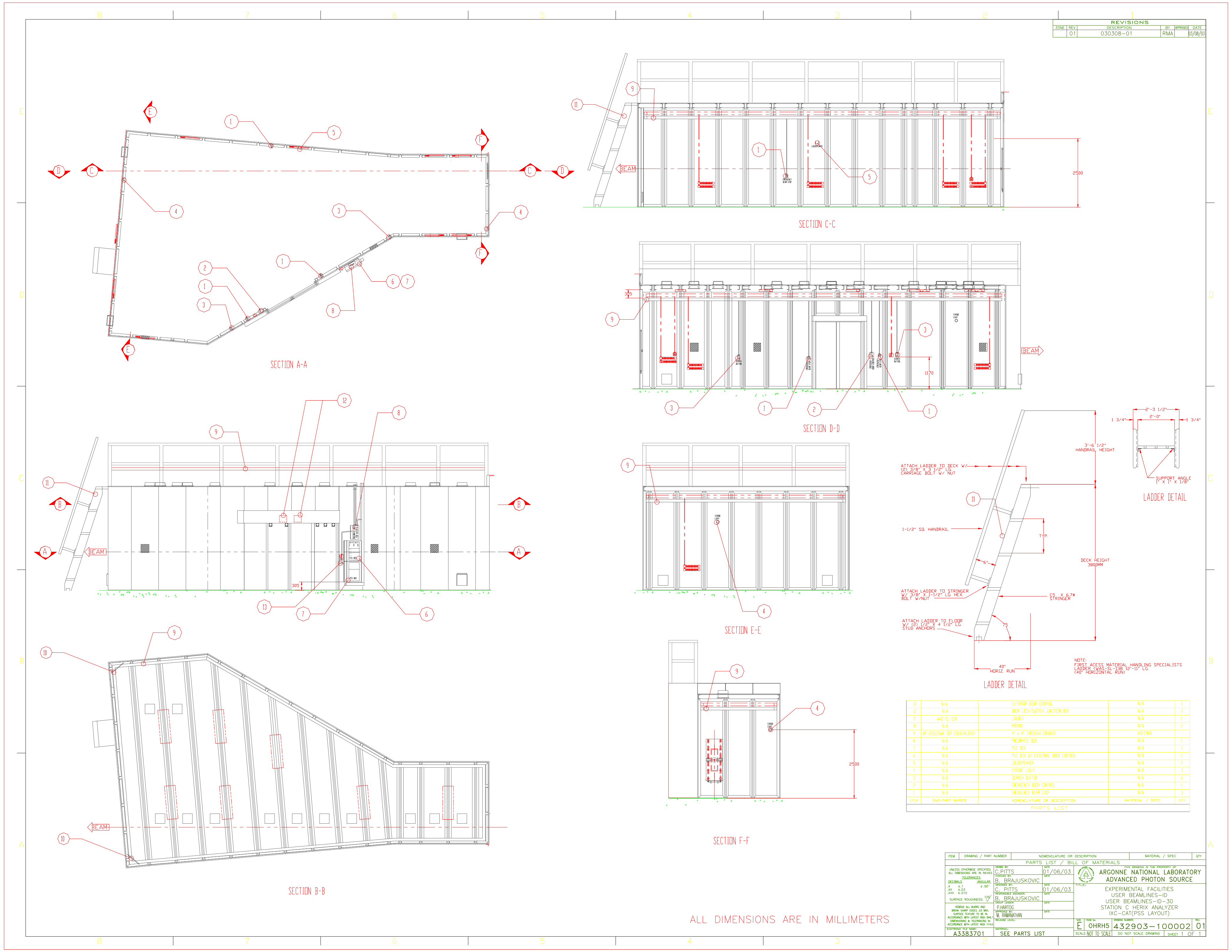


Figure A.14   Personnel safety system layout for station C.



Appendix B. List of Key Beamline Components

Name	Distance (m)	Critical Component	Description
VAT	24.577		Front-end exit valve
PUMP	24.799		Ion pump
MASK	25.123	Critical	Water-cooled exit mask (1x3 mm aperture)
WINDOW	25.661		Be window
PUMP	25.955		Ion pump
K5-20	25.080	Critical	Tungsten bremsstrahlung collimator
VAT	26.358		Beamline isolation valve
PUMP	26.723		Ion pump
L5-94	27.040		White beam slits
L5-94	27.569		White beam slits
CRL	28.096		Be compound refractive lens
PUMP	28.585		Ion pump
VAT	28.849		Vacuum isolation valve
HHM	28.938		High-heat-load monochromator
P5-80	30.400	Critical	White beam stop/ monochromatic shutter
SPOOL	31.737		Shielded transport between stations
WINDOW	32.678		Be window
HRM	33.029		MERIX & HERIX high-resolution monochromator
KB_MERIX	37.400		MERIX KB mirrors
MERIX	39.600		MERIX spectrometer
WINDOW	41.950		Be window
P8-60	41.979	PSS	Monochromatic shutter
SPOOL	42.685		Shielded transport between stations
WINDOW	43.309		Be window
KB_HERIX	43.609		HERIX KB mirrors
HERIX	46.005		HERIX spectrometer

Appendix C. Statement of Work for HHLM

C.1 Introduction and Background Information

A double-crystal monochromator (DCM) is required to select or scan x-ray energies for various experiments on an undulator beamline at the Advanced Photon Source (APS). The DCM consists of a mechanical system for alignment of monochromator components and for selecting or scanning of x-ray energies using two crystals arranged in nondispersive geometry, a vacuum chamber for housing the crystals, a cooling system for preventing damage to the crystal optics under high-thermal-loading conditions, and a support structure. For the IXS-CDT, the total power and power density incident normal on the crystal surface of the DCM will be about 5 kW and 150 W/mm^2, respectively. The crystal optics and the cooling units will be supplied by the APS, while the vendor must provide the vacuum chamber and the mechanical assembly with necessary feedthroughs for cooling requirement. During energy scanning or selection, the exit beam is required to maintain a fixed height offset and a fixed angle with respect to the incident white beam. In particular, most of the experiments planned on the beamline require the angular stability of the exit beam to be better than 0.1 arc second, and, therefore, the mechanical system of the DCM must be carefully designed by proper selection of construction materials and overall structure.

C.2 Scope of Work

This document establishes the requirements for the design, fabrication, inspection, testing, delivery, and installation of the mechanical system, the vacuum system, and a support structure of a DCM for the APS. The complete system must be delivered within nine months of the contract award date. The DCM will house the crystals supplied by the APS and will reside permanently in intense synchrotron beam for the purpose of energy monochromatization. The required DCM as shown in figure C.1 has the bulk of the DCM on the left side of the incident x-ray beam.

The vendor must submit a detailed design report of the DCM with drawings and blueprints (more than 60% completed) within 45 days after the contract is awarded. The design report must also include detailed specifications of major components, a fabrication and testing plan, and a timetable. Acceptance of the design will be made in writing by an official representative of the APS prior to the DCM fabrication. A final design report (with drawings > 95% completed) must be submitted to the APS within 90 days after the contract award date. At the time of delivery, a test report, a DCM operations manual, a full set of final mechanical drawings, all material and component certifications, and all second-source manuals and warranties must be supplied to the APS.

C.3 Applicable Documents

The practices and standards of AVS, ASTM, and ANSI shall be followed when applicable. In particular, the following references shall be used:

- ANSI Y14.5M (1982) Standard for Dimensioning and Tolerancing,

- ASTM F78-79 (1991) Standard Test Methods for Calibration of Helium Leak Detector by Use of Secondary Standards,
- ASTM E498-90 Standard Test Methods for Leaks using the Mass Spectrometer Leak Detector or Residual Gas Analyser in the Tracer Probe Mode.

C.4 Technical Specifications

This section contains technical specifications for the mechanical and vacuum part of the DCM. The overall space requirement of the DCM must be no more than 1.0 m in the direction along the beam (excluding the chamber with a fluorescent screen, if it is detachable, see figure C.2a), +0.4/-1.25 m transverse to the beam, and less than 3 m in height (see figure C.2b). The DCM consists of a support structure, a vacuum chamber, and two crystal mounting stages. Both crystals will be liquid nitrogen cooled. The crystals themselves and the circulation units for the coolant will be supplied by the APS and are not part of this specification. However, the vendor must provide three complete sets (1 set = 1 inlet + 1 outlet) of coolant feedthroughs and transport lines, one set for the first crystal, one set for the second crystal, and a third set for cooling a Compton shield. Preferably, the feedthroughs for cooling the crystals will be on the axis of rotation. The maximum coolant flow rate will be 15 liters/minute for both crystals. The coolant pressure will not exceed 100 psi in all cases.

The undeflected incident beam of maximum size 5 mm (H) x 2 mm (V) is at a height of 1.4 m from the experiment floor. Both crystals must be mounted on a primary rotation stage. The preferred location of the primary rotation axis is on the surface of the first crystal. During energy selection, the overall angle of the two crystals with respect to the incident beam will be changed by a smooth, single rotation of the primary rotation stage. We require that the DCM be capable of tuning the Bragg angle continuously from -1^{o} to 60^{o}.

The source size at the APS is small and the DCM is located at quite a distance ($\approx$54 m) from the source. Both conditions place a very stringent requirement on the relative angular accuracy between the two crystals, because any small angular misalignment will affect the alignment of the downstream optics. Thus the second crystal is required to have two separate highly precise rotational degrees of freedom for fine-tuning the angular offsets with respect to the first crystal. These angular adjustments must possess very high stability, and every design consideration for the DCM should be given to maintaining this angular stability. Also, for the exit beam to maintain a fixed offset in height relative to the incident beam during energy scanning, the second crystal will also need to be translated in the direction normal to the crystal plane. This height offset should be user-adjustable between 1.0-3.5 cm.

C.4.1 Support Structure

Mechanical - The DCM must be mounted on a stable and rigid support structure that also should provide vibration damping. Special attention must be given to the long-term stability (hours to days) of the structure. In particular, the thermal response of the support structure must be minimized. This may be achieved by using materials of low thermal expansion coefficient, passive thermal insulation, increasing the thermal mass, or some other means. However, no active water cooling should be used for the support structure. Also, lifting points and wheels should be equipped on the support structure for moving the entire DCM.

Support Mount - At least five degrees of freedom must be provided for the support structure: vertical translation, horizontal translation transverse to the beam, and the three rotations. This may be accomplished by using 3-point kinematic supports. The horizontal motion transverse to the beam and the vertical motion must be motorized.

Range and Accuracy - The first crystal must be positioned at 1.40 m from the floor with ± 5.0 cm of adjustment for moving the first crystal in and out of the beam. Thus the vertical translation of the support is required to have 10 cm of travel range with 10 micron resolution. The horizontal translation traverse to the beam is needed for aligning the crystals to the incident beam. This motion must also have 10 cm of travel range with 10 micron resolution. Three rotational degrees of freedom are also needed for alignment, and each axis should have ± 5 degrees angular range and 0.1 degree resolution. Among these five degrees of freedom, only the vertical translation and the horizontal translation transverse to the beam must be motorized and remotely controlled.

C.4.2 Vacuum Chamber

Mechanical - The vacuum chamber must be constructed with SS (see figure C.2). All components used inside the vacuum chamber must be HV compatible. Both the input and output beam port must be at least 8" Conflat flanges. In addition to allowing the monochromatic beam to pass through, the output port must be able to allow the incident beam (max. size = 5 mm (H) x 2 mm (V)) to pass through unperturbed when the entire chamber is lowered by 1 cm. A remotely controllable feedthrough must be mounted before the output port for inserting a fluorescent screen to intercept the beam. For examining the fluorescent screen, one viewport must be available. The fluorescent screen will be provided by the APS. A large viewport on at least a 10" Conflat flange must be positioned on one side of the crystal-mounting stages. In addition, a 6" viewport on the top half of the chamber and another on the bottom half must be available for direct viewing of the two crystal surfaces. Quartz windows of zero-profile design must be used for all other viewports installed on the chamber. At least three other 6" and a minimum of eight 2.75" auxiliary ports should also be available. Feedthroughs for at least 10 thermocouples must be available for monitoring the temperatures of the crystals and other components. One ion gauge and one roughing gauge must be provided. Two sets of cooling (liquid nitrogen compatible) feedthroughs and transport lines, each including an inlet and an outlet line, must be provided. In addition, a third set of water-compatible feedthroughs must also be provided. In particular, all cooling feedthroughs must be located at or near the rotation axis of the primary stage (described in Section. 4.3) to minimize the torque on the crystals. All cooling and electrical connections must be strain relieved.

Vacuum - In general, standard UHV practice must be followed (e.g., avoiding any outgassing material and internal/full penetration welds should be used) and clean handling procedures must be followed when assembling the vacuum parts. The final pressure of the entire chamber must be less than 3 x 10^{-7} Torr with all the mechanical parts, crystal mounting stages, and in-vacuum motors installed. The leak rate must be less than $1x10^{-9}$ Torr-l/sec. Residual gas analysis must also be done, and the total pressure from masses above 38 must be less than $5x10^{-10}$ Torr. A Perkin-Elmer ion pump with a total pumping speed of at least 400 l/s must be used. A manual gate valve for at least 8"Conflat flanges must be installed in between the ion pump and the vacuum chamber. The vendor must supply all the vacuum parts up to the flanges, including quartz viewports, blank flanges, electrical in-air mating connectors, and thermocouple feedthroughs, coolant feedthroughs and transport lines, ion pumps and their controller (which has setpoints adjustment), and vacuum gauges (Granville Phillips preferred). The ion pump controller (Perkin-Elmer) must have computer interface, either through an IEEE-488 or RS-232 interface, for remote monitoring purpose. All components inside the vacuum chamber, including all insulations, must be radiation resistant up to at least $1x10^{7}$ rads. Also the vacuum chamber shall be bakable up to 100°C. Only high-vacuum-compatible materials are permitted. In particular, under no circumstances is Teflon allowed anywhere inside the vacuum chamber. Before delivery, the vacuum chamber must be backfilled with dry nitrogen and sealed.

C.4.3 Crystal-Mounting Stages

Coordinate System - The following coordinate system is used for the crystals and is shown in figure C.3:

- x - along the crystal surface, transverse to the diffraction plane
- y - along the normal to the crystal surface
- z - along the crystal surface, in the plane of diffraction
- θ_x - rotation around x-axis (pitch)
- θ_y - rotation around y-axis (yaw)
- θ_z - rotation around z-axis (roll)

General - Because of the long distances encountered at our beamline at the APS, the accuracy and the stability in the angles θ_x and θ_z for the two crystals are of utmost importance. We require that the relative angles between the two crystals to be stable within

$$\Delta\theta_x = |\ \theta_x \text{ (1st crystal)} - \theta_x \text{ (2nd crystal)}\ | < 0.1'' \text{ (arc second)}$$

$$\Delta\theta_z = |\ \theta_z \text{ (1st crystal)} - \theta_z \text{ (2nd crystal)}\ | < 0.5'' \text{ (arc second)}$$

$$\Delta\theta_y = |\ \theta_y \text{ (1st crystal)} - \theta_y \text{ (2nd crystal)}\ | < 20'' \text{ (arc second)}$$

when the crystals are not in motion. This stability shall be maintained over periods of several days (typically a week). Usually, the incident angle on the second crystal may be offset relative to that of the first crystal for the purpose of bandwidth selection or higher harmonic rejection. We still allow the two crystals to be offset. But once the amount of offset is selected (whatever it may be), the offset amount must not deviate by more than the above criterion until the user requests another change. It is essential that all the mechanical motions are decoupled and independent from each other as much as possible. This angular stability between the two crystals should be maintained as much as possible even when the primary rotation is activated. Also, the first crystal must have no mechanical motions other than the rotation caused by the primary rotation stage. The preferred location of all other motions and stages is on the second crystal.

Primary Rotation Stage - During energy selection, the overall angular change for both crystals must be accomplished by a primary rotation stage. For that purpose, both crystals and their mechanical components must be mounted on the primary stage, with the axis of rotation passing preferably through the front surface of the first crystal. The primary rotation stage must employ at least one rotary encoder. Over the 5° to 60° scanning range, the primary rotation must have resolution better than 0.5 arc seconds, repeatability better than 1 arc second, and accuracy better than 10 arc seconds. Both the motor and the encoder must reside outside of the vacuum chamber. The angular range covered by the primary stage must be from -1° to 60°, with 0° being the first crystal lying horizontally and which will be used primarily for alignment purposes. Throughout this angular range, the radial runout of the rotation axis must be less than 5 microns under full loading condition (with all mechanical components, crystal holders, and crystals included). Because the primary rotation stage has to carry the weight of the crystals and all their mechanical components, the rotary axle should be supported at two points as far apart as possible and must be fitted with precision bearings of high loading capacity. All other mechanical motions of the second crystal are riding on this primary stage (see figure C.3). Also, the driving motor must produce sufficient torque and holding force to overcome all tensions and forces created by the coolant transport lines and electrical cables.

y-Translation - For the second crystal, a motorized translation along the normal to the surface is required to maintain a fixed beam offset between the incoming and the outgoing beam during energy scanning. The beam offset must be user selectable between 1.0 cm to 3.5 cm. For that purpose, the y-translation for the second crystal is required to have a travel range of 3.0 cm with an accuracy of 5 microns. The surface of the second crystal must be able to be positioned as close as 0.5 cm directly above the first crystal surface (see figure C.4). In addition, the axis of this y-translation must be movable in the direction parallel to the crystal surface, that is, in the z-direction.

z-Translation - This will be used to reposition the second crystal along z when the beam offset changes. This z-adjustment must be motorized, and an adjustment range of at least 10 cm is required. Ideally, the z-translational range shall be 20 cm (figure C.4). The design for the z-adjustment must not compromise any mechanical tolerance of the y-translation. Also, any y- or z-translation over a range of 1.0 mm must not create angular deviations in the second crystal by more than 2 arc second in either θ_X or θ_Z.

x-Translation - This will be used to reposition the second crystal transverse to the beam direction. This allows selecting a diffraction area on the second crystal in case of non-uniform reflectivity of the second crystal surface. This x-adjustment must be motorized, and an adjustment range of at least 1.0 cm is required. The design for the x-adjustment must not compromise any mechanical tolerance of the y- and z-translation. Also, it is required that any x-, y- or z-translation over a range of 1.0 mm must not create angular deviations in the second crystal by more than 2 arc second in either θ_X or θ_Z.

θ_x for Second Crystal - Remotely controllable fine adjustment in θ_X must be provided for the second crystal. Two ranges are required: a coarse range of $\pm$ 1° and an accuracy of better than 1 arc minute are required, and a fine range of $\pm$ 60 arc second with an accuracy better than 0.1 arc second. The axis of rotation must be located on the front surface of the second crystal. To achieve $\pm$ 0.1 arc second resolution, a PZT device shall be used for this motion. This θ_X rotation axis be parallel to the axis of the primary rotation stage for the two crystals to within 1 arc minute.

θ_z for Second Crystal - Remotely controllable fine adjustment in θ_Z must be provided for the second crystal. A range of $\pm$ 1° and an accuracy of better than 0.5 arc second are required. The axis of rotation must also be located on the front surface of the second crystal. That means the θ_X and the θ_Z axis of the second crystal must intercept at the front surface, and the axes should be orthogonal to each other.

OPTIONAL Rotational Stage

θ_y for Second Crystal - Remotely controllable fine adjustment in θ_Y may be provided for the second crystal. This motion is used for aligning a sagitally focusing second crystal. A range of $\pm$ 1° and an accuracy of better than 20 arc second are required. The axis of rotation must be orthogonal to the surface of the second crystal.

Crystal-Holder Mount - The crystal-holder mounts shall be provided by the vendor. The mounts shall have tapped M5 holes on a 25-mm-square grid pattern. The surfaces shall be precision ground. The crystals and their individual kinematic mounts will be provided by the APS. The vendor must reserve the following clearance space around the crystal (see figure C.5):

first crystal holder	x = 12 cm,	y = 10 cm	z = 15 cm
second crystal holder	x = 12 cm,	y = 15 cm	z = 15 cm
(size of first crystal	x = 12 cm,	y = 7 cm	z = 15 cm)
(size of second crystal	x = 12 cm,	y = 12 cm	z = 15 cm).

The maximum weight of the first crystal and the kinematic mount will not exceed 15 kg, while that for the second crystal will be limited to 8 kg. The interface plate to the kinematic mounts provided by the vendor must have location pins or machined shoulders for precise remounting of the kinematic mounts to within 20 microns in all directions. Coolant feedthroughs and coolant transport lines from the feedthrough to the crystal kinematic mount must be separately provided for the first and the second crystal. Details of the connection between the coolant transport lines and the crystal kinematic mount will be provided by the APS.

Shields - Radiation shields protecting the two crystals against the white beam are part of the crystal holders and will be provided by the APS. However, there will be scattered x-rays present everywhere inside the vacuum chamber, as well as heat radiated to the first crystal. Thus, radiation and heat shielding must be installed around all components as much as possible by the vendor. Special attentions should be given to non-stainless-steel components, mechanical parts requiring lubricants, in-vacuum motors, encoders, limit switches, and cables.

C.4.4 General Guidelines

It should be emphasized that the vacuum system and the crystal-mounting stages of the DCM must be designed to satisfy the relative angular stability requirement between the two crystals ($\Delta\theta_x < 0.1''$, $\Delta\theta_z < 0.5''$, $\Delta\theta_y < 20''$), in addition to meeting other specifications set forth in previous sections. The vendor must supply all the necessary rotation and translation devices including motors, motor drivers, PZTs, and PZT drivers. All the motor drivers must be controllable by an external controller by step and direction (TTL) pulses. Long inchworm-type PZT devices must be avoided, and the range of travel for any PZT device must be limited to no more than 100 μm. The PZT drivers must have computer interface. Motors outside of vacuum should be used as much as possible; in-vacuum motors should be avoided whenever possible. Encoders or transducers must be supplied for each axis of motion. However, in-vacuum encoders do not need to be used for in-vacuum motors if a homing position or limit switch is provided for each motor. It should be emphasized that all components in the vacuum, including encoders, limit switches, cables, insulations, and lubricants, must be able to withstand a radiation dose of at least 1×10^7 rads. Precision machining is expected on all mechanical components. All internal mechanical assemblies must be designed so that disassembly and reassembly can be easily done through the use of location pins or machined shoulders. Survey markings must be available for locating the primary rotation axis and other axes of motions.

C.5 Technical Tasks And Quality Assurance

C.5.1 Design

The vendor shall furnish all personnel and facilities needed to design the DCM vacuum chamber, mechanical system, and support structure. A design report, including a fabrication and testing plan, must be submitted within 45 days after award of contract for review by APS personnel. At that time, the vendor shall furnish all design blueprints and mechanical drawings (> 60% completed) and detailed specifications including quality assurance and list of subcontractors. A timetable for the planned activities shall also be provided. A design review meeting by the APS personnel shall take place within two weeks after the design report is submitted. The APS reserves the right to approve or disapprove any second-source component included in the design. A final design report (with drawings > 95% completed) must be submitted to the APS within 90 days after the contract award date.

C.5.2 Fabrication

Upon written approval by the APS on the proposed design, fabrication, and testing plan, the vendor shall furnish all materials, personnel, facilities, tools, equipment, and services to fabricate, test, and deliver the DCM system to the APS within nine months after award of contract.

C.5.3 Inspection

The APS reserves the right to inspect any and all materials and parts required for completion of this contract. The APS personnel shall have access to the vendor facilities at reasonable times for inspection of the progress of work.

C.5.4 Material Certification

The vendor shall provide the APS with certification of all materials and components used in the fabrication of the DCM system. Use of suspect/counterfeit parts is prohibited according to ANL policy.

C.5.5 Testing

The DCM must be thoroughly tested at the vendor's facilities before delivering to the APS, and the test results must demonstrate that the DCM has met all specifications set forth in Section C.4 of this document. The vendor shall furnish all the necessary personnel, tools, equipment, and facilities for testing the DCM system and components. The APS must approve the vendor's testing plan and procedures before the actual test takes place. The testing may be witnessed by one or more APS representatives.

C.5.6 Delivery

It is the vendor's responsibility to properly package and deliver the DCM to the APS. The vendor must provide a shipping and packaging plan (including customs procedures if necessary) at least one month prior to shipping. Acceptance of the plan will be made in writing by an authorized representative of the APS.

C.5.7 Checkout

The vendor must send at least one of their technical persons to the APS for the unpacking and initial checkout of the DCM. The vendor's representative must verify the conditions and the performance of the DCM upon arrival.

C.5.8 Acceptance Criteria

Acceptance of the DCM will be based on meeting all the specifications set forth in Section C.4 and all the technical tasks described in Sections C.5 of this document or any written revision to this document thereafter agreed upon by both the vendor and the APS. In addition, all the documents listed in Section C.6.1 and hardware listed in Section C.6.2 must be delivered to the APS within nine months from the contract award date. The vendor must demonstrate and document with a certified test report the performance of the DCM.

C.5.9 Modification

After the APS has approved the DCM design, no components of the DCM system shall be modified without the written approval of the APS. The vendor shall report any non-conformance of specifications, drawings, or other contractual requirements on ANL Form 311. Any occurence that affects the fabrication, testing, or delivery schedule shall be reported to the APS within two business days.

C.6 Reports, Data, and Deliverables

The vendor shall deliver the DCM system within nine months from the contract award date. At the time of delivery, the following must have been fully tested and verified:

1. the integrity of the vacuum chamber and the support structure
2. all motions and their tolerances
3. the functionality of any encoder, homing, limit switch, and coolant transport.

Upon arrival of the DCM at the APS, at least one technical personnel of the vendor must come to the APS for the initial checkout.

C.6.1 Deliverable Documents

The vendor must supply the APS with:

1. a design report including drawings (> 60% completed), a fabrication and testing plan, and a schedule of activities, within 45 days of the contract award date,
2. a final design report with drawings > 95% completed within 90 days of the contract award date,
3. written monthly progress reports at the end of each month starting the first month after the contract is awarded,
4. a shipping and packaging plan one month prior to shipping,
5. a full set of the final mechanical drawings and blueprints, prepared in accordance with the ANSI Y14.5M (1982) standard, for all mechanical components, to be delivered with the DCM,
6. operation manuals for the DCM (to be delivered with the DCM),
7. material testing and component certifications (to be delivered with the DCM),
8. all manuals and warranties for second-source components (to be delivered with the DCM),
9. test reports verifying that the mechanical/vacuum/electrical components have met the specifications stated in this Statement of Work (to be delivered with the DCM).

C.6.2 Hardware Deliverables

The vendor must deliver the following hardware to the APS.

1. A support structure including motors and drivers required for the vertical and horizontal translation of the support structure.
2. A vacuum chamber including (a) the necessary quartz viewports, (b) one set of liquid-nitrogen-compatible feedthroughs for the first crystal, (c) one set of liquid-nitrogen-compatible feedthroughs for the second crystal, (d) one set of water-compatible feedthroughs for the Compton shield, (e) a remotely controllable feedthrough for inserting the fluorescent screen, (f) all electrical/thermocouples feedthroughs and connections, (g) blank-off flanges for any unutilized ports, (h) any necessary rail/translation system for moving portions of the vacuum tank during crystal changes.
3. A vacuum pumping system including (a) a Perkin-Elmer ion pump and its controller, (b) a gate valve between the ion pump and the vacuum chamber, (c) a Granville-Phillips ion gauge and a roughing gauge with a controller that has

setpoint capability. Computer interfaces for the ion pump controller with setpoints must also be included.

4. Crystal-mounting stages including (a) a primary rotation stage assembly with motor, its driver and rotary encoders, (b) all other crystal rotation/translation stages with motors, drivers, and encoders/transducers, (c) all cables inside and outside of the vacuum system necessary to power the stages and encoders/transducers, (d) any PZT device with driver and transducer, (e) all the adapters, and mounting or alignment pieces needed to achieve the required motions and their tolerance, (f) two interface plates to the crystal kinematic mounts, (g) radiation and heat shielding around any in-vacuum motor, encoder or limit switch, and cables.

C.7 Special Considerations

The crystals and their kinematic mounts will be supplied by the APS. Details of the crystal-mount geometry and the coolant connection will be provided to the vendor within two months after the contract award date. The connections from the external coolant circulation units to the coolant feedthroughs on the DCM vacuum chamber will also be specified at that time.

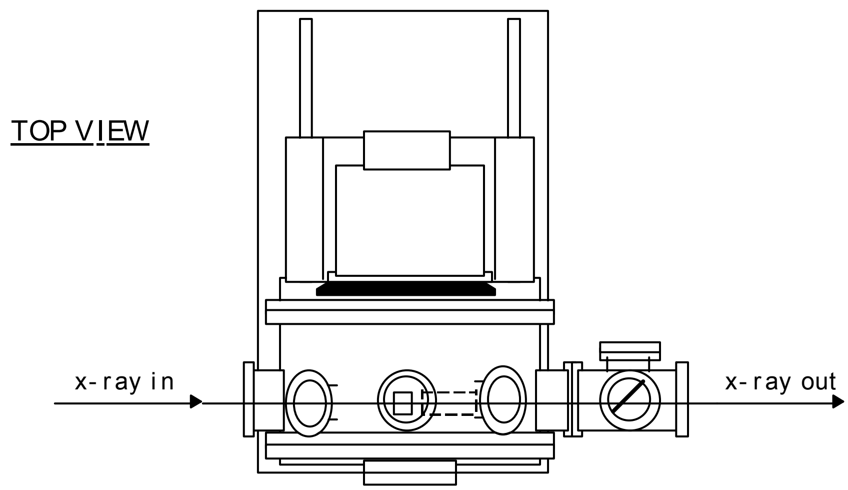


Figure. C.1 *Top view of the DCM's orientation with respect to the incoming x-ray beam.*

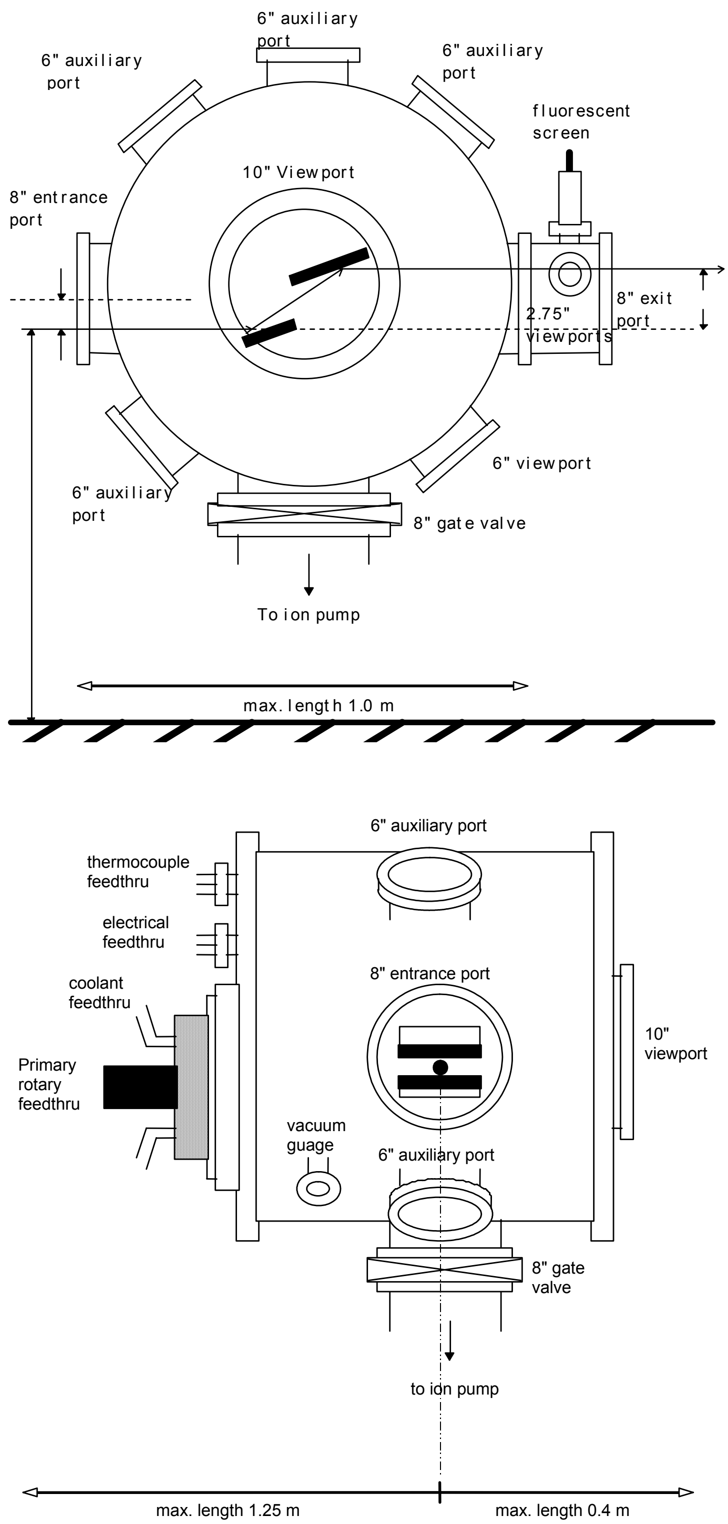


Figure C.2. *(a) Elevation view of a possible configuration for the stainless steel vacuum chamber, showing the major vacuum components that are required. Size (O.D.) of standard Conflat flanges are shown. (b) Downstream view of the vacuum chamber.*

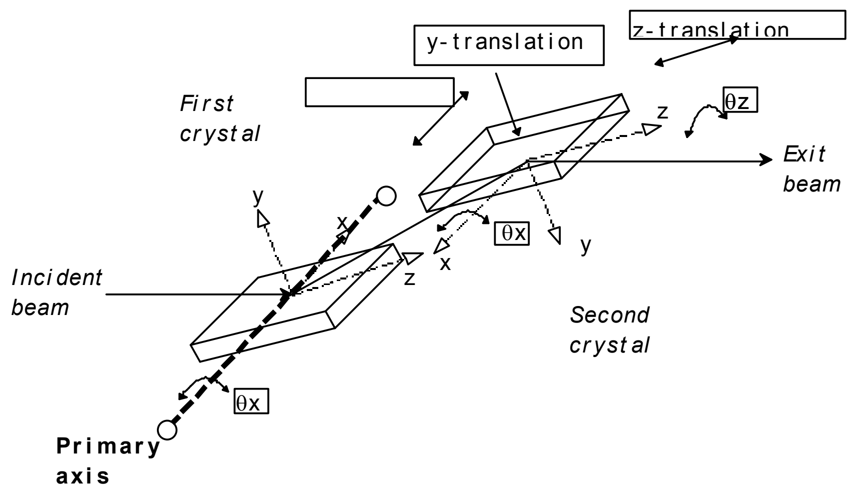


Figure C.3. *Coordinate system for the two crystals. The (six) mechanical motions required on the crystals are labeled in boxes. Both crystals are riding on the primary rotation stage whose axis passes through the surface of the first crystal.*

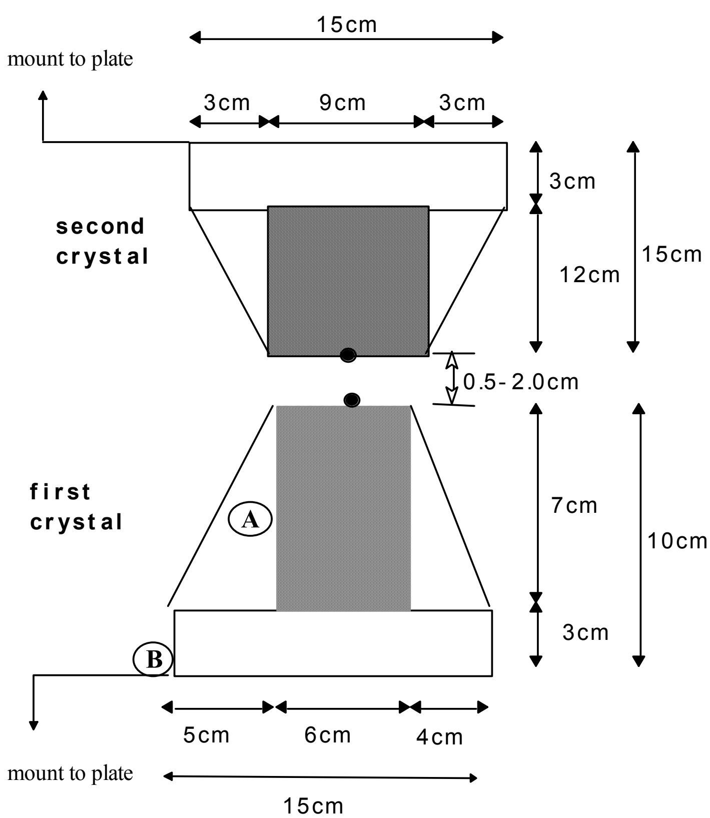


Figure C.4. *Schematic view from entrance port of the crystals and the crystal mounts (not to scale), showing the maximum clearance required. The y-translation must position the second crystal surface between 0.5 cm to 2.0 cm above the first crystal surface.*

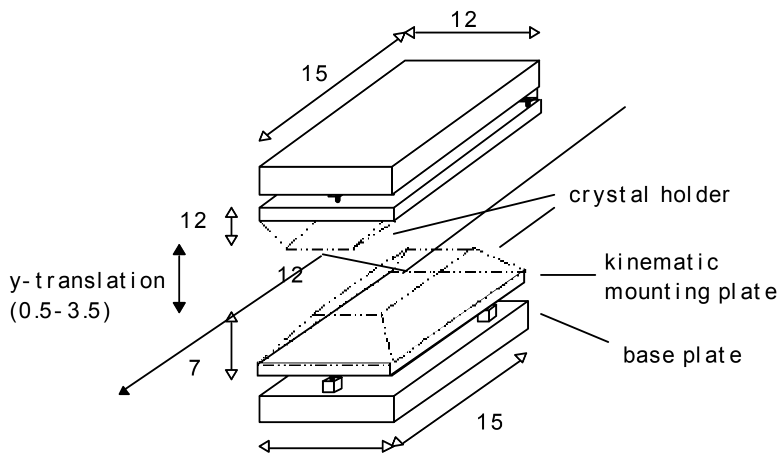


Figure C.5. *Side view of a possible arrangement of the crystals and kinematic mounts (not to scale). Mechanical components interfaced to the kinematic mounts must be supplied by the vendor. The crystals and the kinematic mounts will be supplied by the APS. All numbers are in cm.*

Appendix D. Statement of Work for Mirrors

D.1 Kirkpatrick-Baez Mirror Systems: Design considerations

The basic concept is to have two independent K-B mirror systems that will be used when either the MERIX or the HERIX spectrometer is in operation. Therefore each mirror system can be optimized for its energy range (5-12 keV for MERIX and 20-26 keV for HERIX) and the precise sample positions. To minimize the focal spot, but also because of space limitations, the aspect ratios are extremely high (up to 42:1), leading to short bending radii of less than 1 km. However, since there is very little flexibility required, the mirrors can be pre-shaped to the required radii. The focusing gain of elliptical bending is about a factor of two for each mirror and is therefore quite important. The downstream sequence for both mirror systems is horizontal-vertical focusing. In this way, the aspect ratio of the horizontal mirrors is a little relaxed without requiring more space in the stations. This makes the fabrication of the horizontal mirrors feasible without compromising too much on the slope errors.

The lengths of the mirrors were chosen to be about 4 sigma of the beam footprint (95% transmission) for the currently lowest emittance mode at the APS. We chose bimorph (adaptive) mirrors over conventionally bent mirrors because of the exceptional performance of the bimorph mirrors in HP-CAT, which can even correct distortions in the beam profile from, e.g., the diamond crystals in the monochromator. In addition, the bimorph mirrors are of more compact design, which is a plus considering the space limitations in the B and C stations (see figure D.1).

Both mirror systems will be in vacuum tanks with both horizontal and vertical mirrors in one unit and beryllium windows on each side. The MERIX mirrors will have gate valves with integrated beryllium windows to minimize the loss at 5 keV operation. All mirrors will be fully motion controlled by step motors and by additional piezo actuators for the pitch angles for beam-position corrections. Since the temperature in the station will be stabilized, there is no need for active temperature stabilization of the mirrors.

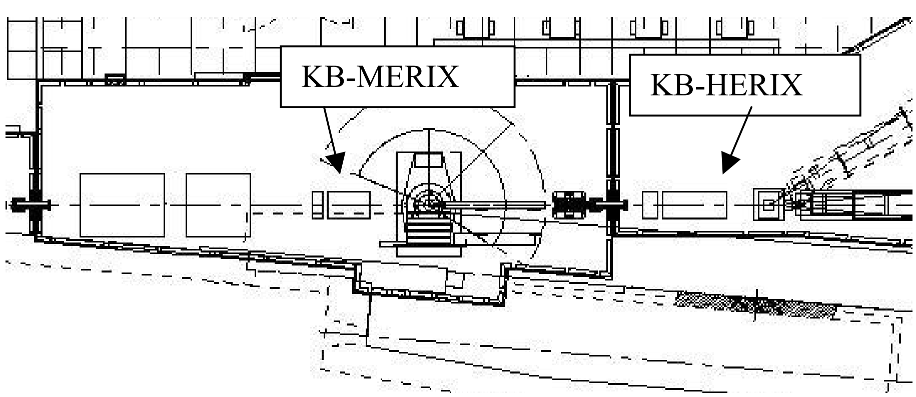


Figure D.1. *Location of K-B mirrors in stations B and C.*

D.2 Source Parameters Used in Calculations

eta = 2.3 nmrad, coupling k_{xy} = 0.025
sigma x = 266 micron, FWHM = 625 micron
sigma y = 12.9 micron FWHM = 30.3 micron
sigma x' = 10.9 μrad FWHM = 25.6 μrad
sigma y' = 4.5 μrad FWHM = 10.57 μrad

sigma r = 1 micron
sigma r' = 3.2 μrad (25 keV), 4.5 μrad (10 keV)

10 keV:
SIGMA x' = 11.8 μrad FWHM = 28 μrad
SIGMA y' = 6.4 μrad FWHM = 15 μrad

25 keV:
SIGMA x' = 11.4 μrad FWHM = 27 μrad
SIGMA y' = 5.5 μrad FWHM = 13 μrad

D.3 Choice of Coatings

MERIX:
Assumed values for surface quality: 3 $Å^{-1}$ rms
Coating: Pd or Rh
Reflectivities for ± 1 mrad

Alpha (μrad)	3.0	3.5	4.0	4.5	5	average
Reflectivity 5 keV	.911	.897	.881	.866	.848	.88
9 keV	.931	.917	.900	.881	.858	.90
12 keV	.933	.915	.891	.858	.793	.87
15 keV	.930	.901	.842	.320	.10	(.62)

Average reflectivity around 88% for alpha = 4 ± 1 mrad for 5-12 keV
For 15 keV alpha should be around 3 mrad

HERIX:
Assumed values for surface quality: 3 $Å^{-1}$ rms
Coating: Pt
Reflectivities for ± 0.5 mrad

Alpha (μrad)	1.9	2.2	2.4	2.6	2.9	average
Reflectivity 21 keV	.901	.877	.862	.844	.807	.858
25.7 keV	.900	.871	.850	.822	.759	.840

Average reflectivity around 85% for alpha = 2.4 ± 0.5 mrad

D.4 Mirror Specifications and Focus Sizes

Horizontal mirror MERIX:

(active) length:	0.6 m	
position:	37.9 m	
sample:	39.6 m	
focus distance:	1.7 m	
aspect ratio:	22 : 1	
nominal bending radius:	813 m (4 mrad)	
	1084 m (3 mrad)	
local bending radius:	675-949 m (4mrad)	
	900-1266 m (3mrad)	
range of incident angles:	4 ± 0.37 µrad	
coating:	Pd	
geometrical focus size:	28.4 micron	
SHADOW simulation:	focus: 27 micron	
	only spherical bending: 47 micron	
	lost beams:	2.3% (4mrad), 7.4% (3mrad)
estimated focus with 5 µrad slope error:		44 micron

Vertical mirror MERIX:

(active) length:	0.3 m	
position:	38.4 m	
sample:	39.6 m	
focus distance:	1.2 m	
aspect ratio:	32 : 1	
nominal bending radius:	581 m (4 mrad)	
	775 m (3 mrad)	
local bending radius:	511-652 (4mrad)	
	681-869 (3mrad)	
range of incident angles:	4 ±0.25 µrad	
coating:	Pd	
geometrical focus size:	0.95 micron	
SHADOW simulation:	focus: 1 micron	
	only spherical bending: 15.5 micron	
	lost beams:	1.3% (4mrad), 5.1% (3mrad)
estimated focus with 2 µrad slope error:		9.6 micron

Horizontal mirror HERIX:

(active) length:	0.9 m
position:	44.2 m
sample: 46.0 m	
focus distance:	1.8 m
aspect ratio:	24.5 : 1
nominal bending radius:	1440 m
local bending radius:	1090 – 1880 m
range incident angles:	2.4 ±0.31 mrad

coating:	Pt	
geometrical focus size:	25.5 micron	
SHADOW simulation:	focus: 25.1 micron (no slope error),	
only spherical bending: 60 micron		
	lost beams:	5.5%
estimated focus with 5 μrad slope error:		44 micron

Vertical mirror HERIX:

(active) length:	0.45 m
position:	44.925 m
sample:	46.0 m
focus distance:	1.075 m
aspect ratio:	42 : 1
nominal bending radius:	875 m
local bending radius:	695 – 1050 m
range of incident angles:	2.4 ± 0.26 mrad
coating:	Pt
geometrical focus size:	0.72 micron
SHADOW simulation:	focus: 0.78 micron, only spherical: 17 microns
	lost beams: 2.6%
estimated focus with 2 μrad slope error:	8.6 micron

Estimate on extreme bending cases

- source point is moved 2.75 m: relative change of radius < 1%
- Beryllium lens in front of HHLM: relaxation by < 5 %

D.5 Efficiencies

Transmission through **HERIX** pair: (20-26 keV)

Reflectivity horizontal	0.85	
Beam cut off	0.945	
Reflectivity vertical	0.85	
Beam cut off	0.974	
Total transmission:	**0.67**	
Air transmission 21 keV	0.89	(1.7 m length)
Helium	0.995	

Transmission through **MERIX** pair: (5-12 keV)

Reflectivity horizontal	0.88	
Beam cut off	0.977	
Reflectivity vertical	0.88	
Beam cut off	0.987	
Total transmission:	**0.75**	
Air transmission 9 keV	0.47	(1.25 m length)
Helium	0.994	
Helium 5 keV	0.986	

D.6 SHADOW Simulation

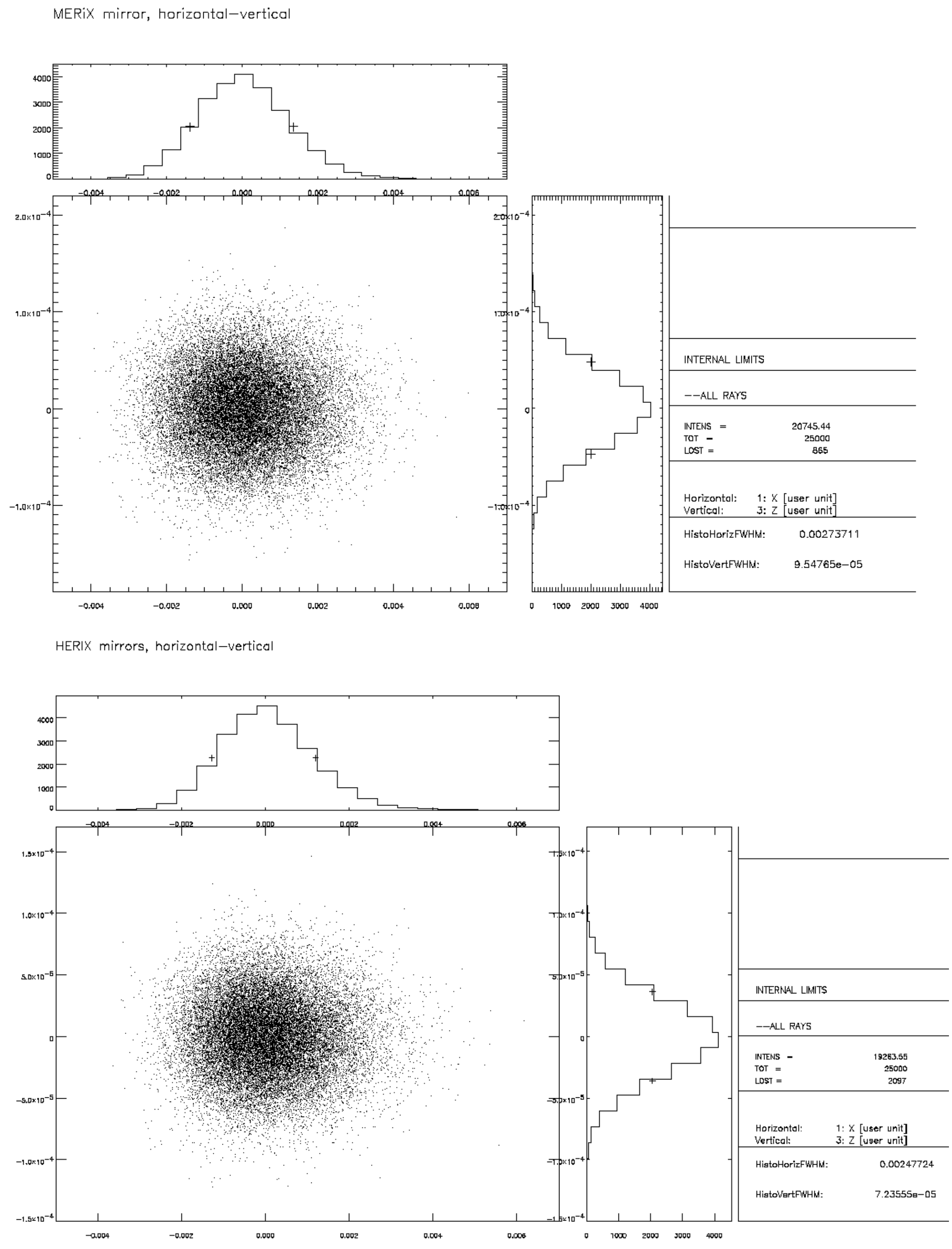
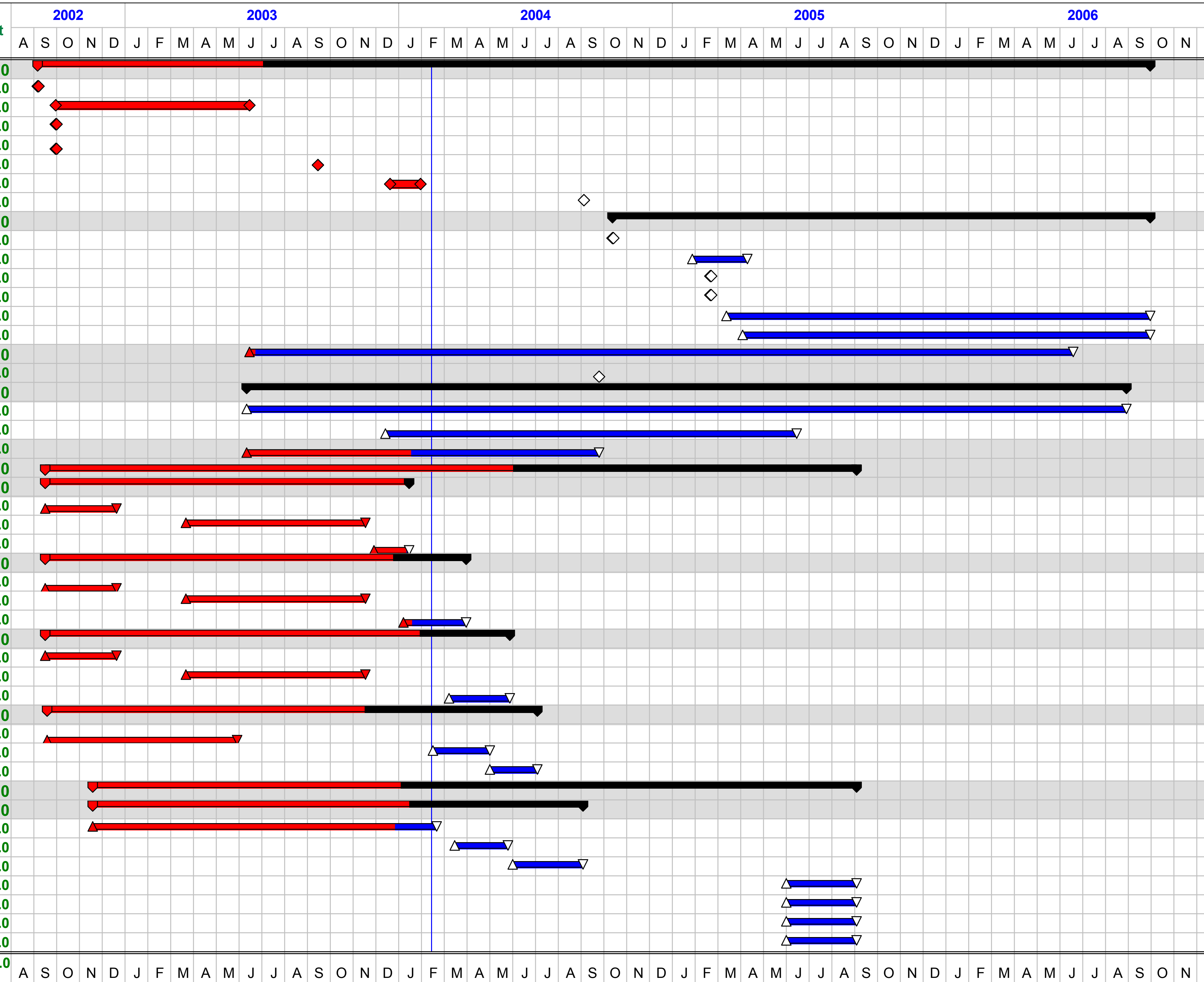


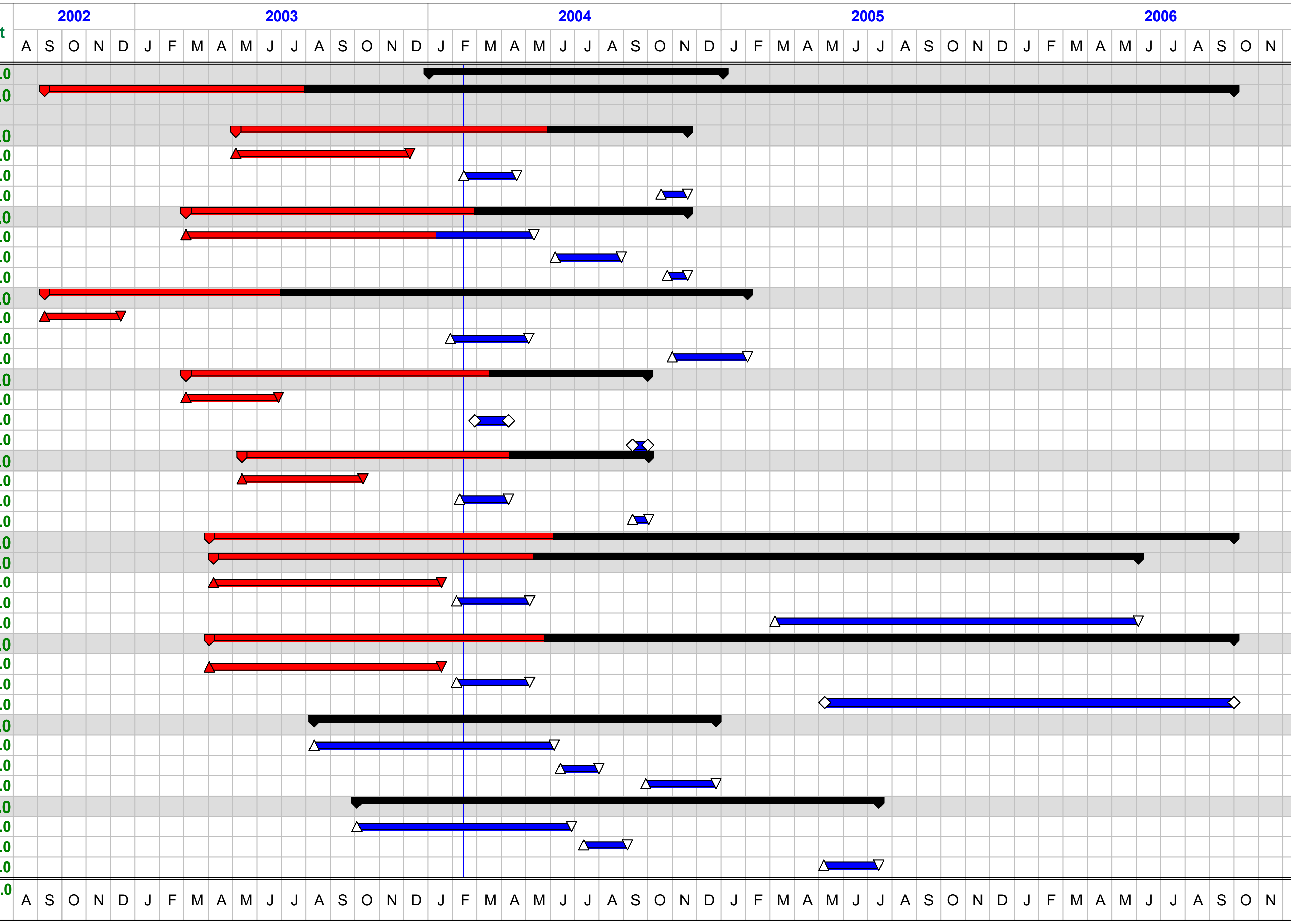
Figure D.2. *Ray-tracing simulations of the two mirror systems performed with the simulation packet SHADOW. Slope errors are not included. Units are in cm.*

Appendix E. Overview of WBS and Major Milestones

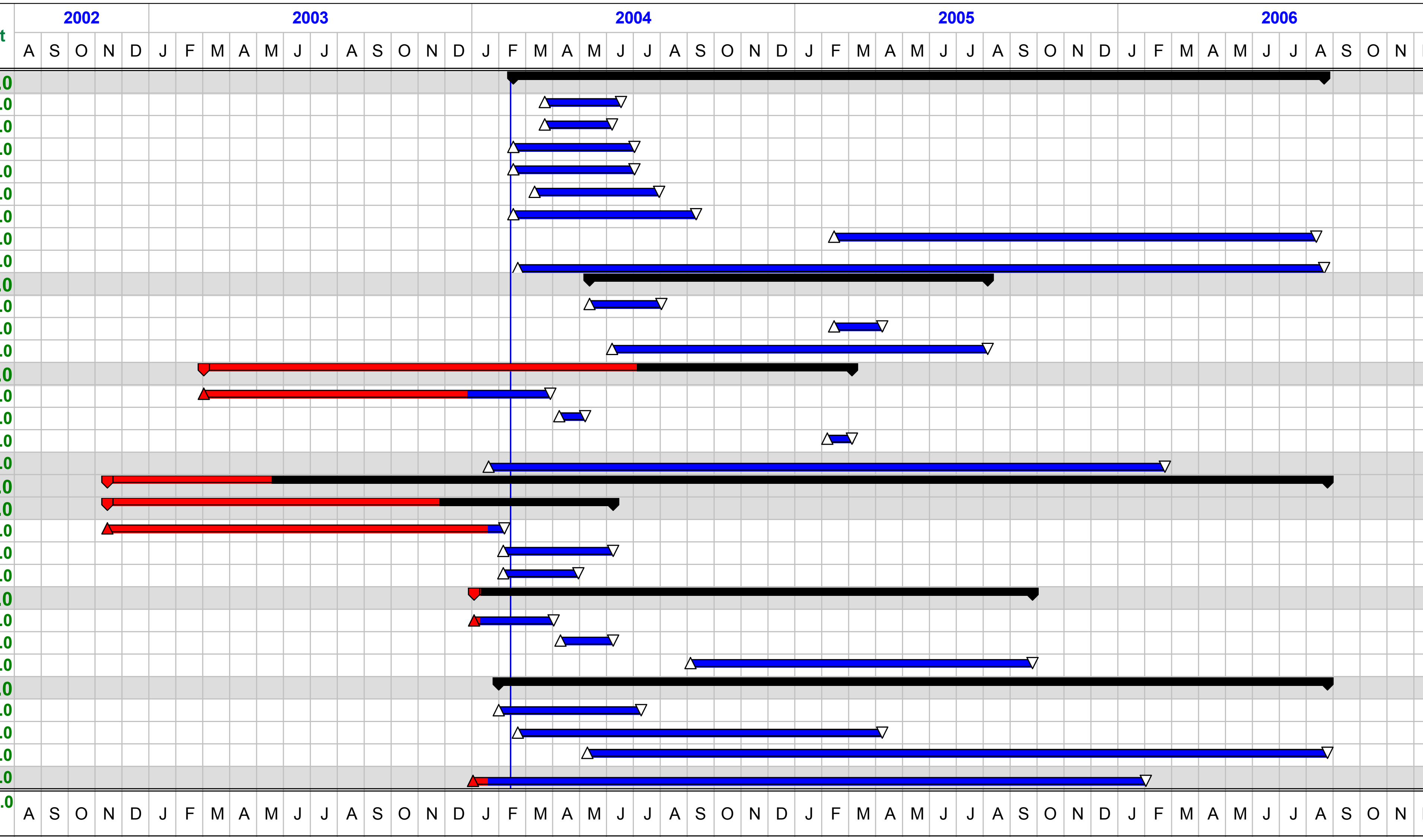
WBS	Activity Name	Start Date	Finish Date	Total Budget K$
IXS-1.4.3.30.1	Planning	9/6/02	9/29/06	0.0
IXS-1.4.3.30.1.1	CDR	9/6/02	9/6/02	0.0
IXS-1.4.3.30.1.2	Management Plan	9/30/02	6/14/03	0.0
IXS-1.4.3.30.1.3	Safety Plan	9/30/02	9/30/02	0.0
IXS-1.4.3.30.1.4	Cost & Schedule Plan	9/30/02	9/30/02	0.0
IXS-1.4.3.30.1.5	MOU	9/15/03	9/15/03	0.0
IXS-1.4.3.30.1.6	PDR	12/21/03	1/30/04	0.0
IXS-1.4.3.30.1.7	FDR	9/4/04	9/4/04	0.0
IXS-1.4.3.30.1.8	Commissioning	10/13/04	9/29/06	0.0
IXS-1.4.3.30.1.8.1	Shielding Verification Station A	10/13/04	10/13/04	0.0
IXS-1.4.3.30.1.8.2	Commissioning Station A Optics	1/28/05	4/9/05	0.0
IXS-1.4.3.30.1.8.3	Shielding Verification Station B	2/20/05	2/20/05	0.0
IXS-1.4.3.30.1.8.4	Shielding Verification Station C	2/20/05	2/20/05	0.0
IXS-1.4.3.30.1.8.5	Commissioning Station B	3/13/05	9/29/06	0.0
IXS-1.4.3.30.1.8.6	Commissioning Station C	4/3/05	9/29/06	0.0
IXS-1.4.3.30.2	SR Modifications	6/14/03	6/18/06	0.0
IXS-1.4.3.30.3	Straight Section Vacuum Chamber (5m)		9/24/04	0.0
IXS-1.4.3.30.4	Insertion Devices	6/11/03	8/28/06	0.0
IXS-1.4.3.30.4.1	Undulator A	6/11/03	8/28/06	0.0
IXS-1.4.3.30.4.2	Superconducting Undulator	12/14/03	6/14/05	0.0
IXS-1.4.3.30.5	Front End	6/11/03	9/24/04	0.0
IXS-1.4.3.30.6	Beamline Stations & Infrastructure	9/16/02	9/3/05	1,390.0
IXS-1.4.3.30.6.1	Station A	9/16/02	1/15/04	210.0
IXS-1.4.3.30.6.1.1	Design	9/16/02	12/20/02	0.0
IXS-1.4.3.30.6.1.2	Procurement	3/21/03	11/16/03	210.0
IXS-1.4.3.30.6.1.3	Installation	11/28/03	1/15/04	0.0
IXS-1.4.3.30.6.2	Station B	9/16/02	3/31/04	319.0
IXS-1.4.3.30.6.2.1	Design	9/16/02	12/20/02	0.0
IXS-1.4.3.30.6.2.2	Procurement	3/21/03	11/16/03	319.0
IXS-1.4.3.30.6.2.3	Installation	1/7/04	3/31/04	0.0
IXS-1.4.3.30.6.3	Station C	9/16/02	5/28/04	411.0
IXS-1.4.3.30.6.3.1	Design	9/16/02	12/20/02	0.0
IXS-1.4.3.30.6.3.2	Procurement	3/21/03	11/16/03	411.0
IXS-1.4.3.30.6.3.3	Installation	3/7/04	5/28/04	0.0
IXS-1.4.3.30.6.4	Beamline Utilities	9/18/02	7/3/04	150.0
IXS-1.4.3.30.6.4.1	Design	9/18/02	5/30/03	0.0
IXS-1.4.3.30.6.4.2	Procurement	2/15/04	4/30/04	150.0
IXS-1.4.3.30.6.4.3	Installation	5/1/04	7/3/04	0.0
IXS-1.4.3.30.6.5	Work Area Enclosure	11/18/02	9/3/05	225.0
IXS-1.4.3.30.6.5.1	Enclosure	11/18/02	9/3/04	140.0
IXS-1.4.3.30.6.5.1.1	Design	11/18/02	2/20/04	0.0
IXS-1.4.3.30.6.5.1.2	Procurement	3/15/04	5/25/04	140.0
IXS-1.4.3.30.6.5.1.3	Installation	6/1/04	9/3/04	0.0
IXS-1.4.3.30.6.5.2	Furniture	6/1/05	9/3/05	50.0
IXS-1.4.3.30.6.5.3	Computers	6/1/05	9/3/05	20.0
IXS-1.4.3.30.6.5.4	Printers	6/1/05	9/3/05	10.0
IXS-1.4.3.30.6.5.5	TV Monitors	6/1/05	9/3/05	5.0
				6,450.0



WBS	Activity Name	Start Date	Finish Date	Total Budget K$
IXS-1.4.3.30.6.6	Beamline Staff (MERIX)	1/2/04	1/3/05	75.0
IXS-1.4.3.30.7	Beamline Optics	9/9/02	9/30/06	2,019.0
IXS-1.4.3.30.7.1	Filter...			
IXS-1.4.3.30.7.2	White Beam Slits	5/5/03	11/19/04	44.0
IXS-1.4.3.30.7.2.1	Design	5/5/03	12/8/03	0.0
IXS-1.4.3.30.7.2.2	Procurement	2/14/04	4/20/04	44.0
IXS-1.4.3.30.7.2.3	Installation	10/18/04	11/19/04	0.0
IXS-1.4.3.30.7.3	Focusing Lens	3/3/03	11/19/04	44.0
IXS-1.4.3.30.7.3.1	Design	3/3/03	5/11/04	0.0
IXS-1.4.3.30.7.3.2	Procurement	6/7/04	8/30/04	44.0
IXS-1.4.3.30.7.3.3	Installation	10/25/04	11/19/04	0.0
IXS-1.4.3.30.7.4	Primary Monochromator	9/9/02	2/3/05	400.0
IXS-1.4.3.30.7.4.1	Design	9/9/02	12/13/02	0.0
IXS-1.4.3.30.7.4.2	Procurement	1/30/04	5/5/04	400.0
IXS-1.4.3.30.7.4.3	Installation	11/1/04	2/3/05	0.0
IXS-1.4.3.30.7.5	Integral Shutter	3/3/03	10/1/04	50.0
IXS-1.4.3.30.7.5.1	Design	3/3/03	6/27/03	0.0
IXS-1.4.3.30.7.5.2	Procurement	2/28/04	4/10/04	50.0
IXS-1.4.3.30.7.5.3	Installation	9/12/04	10/1/04	0.0
IXS-1.4.3.30.7.6	Monochromatic Shutter	5/12/03	10/1/04	50.0
IXS-1.4.3.30.7.6.1	Design	5/12/03	10/10/03	0.0
IXS-1.4.3.30.7.6.2	Procurement	2/9/04	4/9/04	50.0
IXS-1.4.3.30.7.6.3	Installation	9/12/04	10/1/04	0.0
IXS-1.4.3.30.7.7	Monochromatic Mirrors	4/2/03	9/30/06	1,100.0
IXS-1.4.3.30.7.7.1	MERIX Mirror	4/7/03	6/3/06	550.0
IXS-1.4.3.30.7.7.1.1	Design	4/7/03	1/17/04	0.0
IXS-1.4.3.30.7.7.1.2	Procurement	2/6/04	5/6/04	550.0
IXS-1.4.3.30.7.7.1.3	Installation	3/7/05	6/3/06	0.0
IXS-1.4.3.30.7.7.2	HERIX Mirror	4/2/03	9/30/06	550.0
IXS-1.4.3.30.7.7.2.1	Design	4/2/03	1/17/04	0.0
IXS-1.4.3.30.7.7.2.2	Procurement	2/6/04	5/6/04	550.0
IXS-1.4.3.30.7.7.2.3	Installation	5/9/05	9/30/06	0.0
IXS-1.4.3.30.7.8	Support Tables (3)	8/11/03	12/25/04	20.0
IXS-1.4.3.30.7.8.1	Design	8/11/03	6/5/04	0.0
IXS-1.4.3.30.7.8.2	Procurement	6/13/04	7/31/04	20.0
IXS-1.4.3.30.7.8.3	Installation	9/28/04	12/25/04	0.0
IXS-1.4.3.30.7.9	Optical Tables	10/3/03	7/15/05	90.0
IXS-1.4.3.30.7.9.1	Design	10/3/03	6/26/04	0.0
IXS-1.4.3.30.7.9.2	Procurement	7/12/04	9/5/04	90.0
IXS-1.4.3.30.7.9.3	Installation	5/7/05	7/15/05	0.0
				6,450.0



WBS	Activity Name	Start Date	Finish Date	Total Budget K$
IXS-1.4.3.30.7.10	Vacuum Hardware	2/16/04	8/22/06	150.0
IXS-1.4.3.30.7.10.1	Ion pumps & controllers	3/23/04	6/16/04	45.0
IXS-1.4.3.30.7.10.2	Ion gauges & controllers	3/23/04	6/7/04	10.0
IXS-1.4.3.30.7.10.3	Inline valves	2/16/04	7/2/04	10.0
IXS-1.4.3.30.7.10.4	Roughing valves	2/16/04	7/2/04	5.0
IXS-1.4.3.30.7.10.5	Bellows	3/11/04	7/30/04	10.0
IXS-1.4.3.30.7.10.6	Shielded spool transports	2/16/04	9/10/04	10.0
IXS-1.4.3.30.7.10.7	Pumping stations	2/14/05	8/12/06	20.0
IXS-1.4.3.30.7.10.8	Miscellaneous vacuum hardware	2/21/04	8/22/06	15.0
IXS-1.4.3.30.7.10.9	Beamline rough vacuum system	5/12/04	8/5/05	25.0
IXS-1.4.3.30.7.10.9.1	Design	5/12/04	8/1/04	0.0
IXS-1.4.3.30.7.10.9.2	Procurement	2/14/05	4/8/05	25.0
IXS-1.4.3.30.7.10.9.3	Installation	6/7/04	8/5/05	0.0
IXS-1.4.3.30.7.11	Be Windows	3/2/03	3/4/05	20.0
IXS-1.4.3.30.7.11.1	Design	3/2/03	3/29/04	0.0
IXS-1.4.3.30.7.11.2	Procurement	4/8/04	5/7/04	20.0
IXS-1.4.3.30.7.11.3	Installation	2/7/05	3/4/05	0.0
IXS-1.4.3.30.7.12	Student	1/21/04	2/22/06	51.0
IXS-1.4.3.30.8	General Instrumentation	11/15/02	8/25/06	511.0
IXS-1.4.3.30.8.1	PSS	11/15/02	6/8/04	60.0
IXS-1.4.3.30.8.1.1	Design	11/15/02	2/6/04	0.0
IXS-1.4.3.30.8.1.2	Procurement	2/6/04	6/8/04	60.0
IXS-1.4.3.30.8.1.3	Installation	2/6/04	4/29/04	0.0
IXS-1.4.3.30.8.2	EPS	1/4/04	9/25/05	33.0
IXS-1.4.3.30.8.2.1	Design	1/4/04	4/2/04	0.0
IXS-1.4.3.30.8.2.2	Procurement	4/9/04	6/8/04	33.0
IXS-1.4.3.30.8.2.3	Installation	9/5/04	9/25/05	0.0
IXS-1.4.3.30.8.3	Controls	2/1/04	8/25/06	300.0
IXS-1.4.3.30.8.3.1	Design	2/1/04	7/9/04	0.0
IXS-1.4.3.30.8.3.2	Procurement	2/22/04	4/8/05	300.0
IXS-1.4.3.30.8.3.3	Installation	5/10/04	8/25/06	0.0
IXS-1.4.3.30.8.4	Drafting	1/2/04	2/2/06	118.0
				6,450.0



WBS	Activity Name	Start Date	Finish Date	Total Budget K$
IXS-1.4.3.30.9	MERIX Instrumentation	5/12/03	8/4/06	955.7
IXS-1.4.3.30.9.1	Spectrometer	5/10/04	8/6/04	495.0
IXS-1.4.3.30.9.2	Optical Table	2/21/05	10/7/05	66.0
IXS-1.4.3.30.9.3	Detectors	2/21/05	10/7/05	22.0
IXS-1.4.3.30.9.4	Monochromator	5/12/03	10/29/05	200.0
IXS-1.4.3.30.9.5	Analysers	2/21/05	10/7/05	33.0
IXS-1.4.3.30.9.6	Monochromator crystals	2/16/04	9/24/04	33.0
IXS-1.4.3.30.9.7	Sample cell & translation	2/14/05	8/5/05	11.0
IXS-1.4.3.30.9.8	Beam transport	2/14/05	8/5/05	22.0
IXS-1.4.3.30.9.9	Riso slits	2/14/05	8/5/05	22.0
IXS-1.4.3.30.9.10	Displex cryostat	2/13/06	8/4/06	33.0
IXS-1.4.3.30.9.11	Turbo pump	2/13/06	8/4/06	16.5
IXS-1.4.3.30.9.12	Small pumps	2/13/06	8/4/06	2.2
IXS-1.4.3.30.10	HERIX Instrumentation	11/18/02	7/1/06	949.6
IXS-1.4.3.30.10.1	Main structure of spectrometer	5/12/04	11/14/04	77.0
IXS-1.4.3.30.10.2	CZT detector	5/10/04	11/12/04	193.6
IXS-1.4.3.30.10.3	Monochromator	5/18/03	3/18/05	250.0
IXS-1.4.3.30.10.4	Analysers	5/17/05	8/4/05	200.0
IXS-1.4.3.30.10.5	Vacuum chamber	9/15/04	12/13/04	44.0
IXS-1.4.3.30.10.6	Sample motion goniometers	11/18/02	3/7/03	44.0
IXS-1.4.3.30.10.7	Sample slit motion detector	5/18/05	9/4/05	16.5
IXS-1.4.3.30.10.8	Keithley multimeter	5/14/05	7/20/05	11.0
IXS-1.4.3.30.10.9	Motor cables	5/12/05	8/29/05	16.5
IXS-1.4.3.30.10.10	Vacuumpumps	2/13/06	6/9/06	33.0
IXS-1.4.3.30.10.11	Sample table	2/14/06	7/1/06	55.0
IXS-1.4.3.30.10.12	VME crate for analyser motors	2/16/04	8/13/04	9.0
IXS-1.4.3.30.11	Lab Office Module	6/5/06	9/29/06	258.5
IXS-1.4.3.30.11.1	Office build out	6/5/06	9/29/06	77.0
IXS-1.4.3.30.11.2	Office furniture	8/1/06	9/29/06	33.0
IXS-1.4.3.30.11.3	Office equipment	8/1/06	9/29/06	33.0
IXS-1.4.3.30.11.4	Wet lab	6/5/06	9/29/06	60.5
IXS-1.4.3.30.11.5	Dry lab	6/5/06	9/29/06	55.0
IXS-1.4.3.30.12	Contingency	10/1/02	9/29/06	366.2
				6,450.0